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The Scattering Of Positrons By Hydrogen Atoms

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THE SCATTERING OF POSITRONS BY HYDROGEN ATOMS

by

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ABSTRACT

The S-wave scattering of positrons by hydrogen atoms in the energy region up to the first excitation threshold of hydrogen is studied. In the upper part of this energy region, the two reactions

$$e^+ + H(1s) \rightarrow e^+ + H(1s)$$
$$\rightarrow Ps(1s) + H^+$$

are possible, giving the open channels. The closed channel part of the wave function is approximated by a sum of short range correlation terms. Equations for the scattering functions and the coefficients of the expansion in the correlation terms are obtained variationally. The formulation satisfies the bound primciple: the phase shift and the eigen phases are lower bound estimates to the exact values.

For energies in the elastic scattering region, the phase shifts are in very good agreement with those from the accurate calculation of Bhatia et al[1]. In the inelastic region, this thesis presents new results, which by the bound principle, are better than previous results.

A detailed hunt for resonances in the energy below the n=2 excitation threshold of hydrogen produced negative results despite of the claim by Mittleman[2] of the existence of an infinite series of resonance. As a test on the flexibility and capability of the trial wave function to

produce a resonance, the same wave function without the positronium channel term is used to study the electron-hydrogen problem without exchange. A resonance is reproduced with position very close to that obtained by Burke and Schey[3] using a three-state approximation. In addition, at low energy, violent variations in phase shift are observed. An independent calculation, using a five-state close coupling approximation, produces similar results.

The coupled integro-differential equations for the scattering functions are first converted to coupled integral equations, and the values of the functions at a specified net of points are obtained by solving a system of approximating linear algebraic equations. Numerical integrations are carried out using the Gauss-Legendre quadrature, if the limits are finite, or the Gauss-Laguerre formula, when the upper limit is infinite. These decrease the dimension of the system of linear equations to 75x75, a manageable and economical size. Most of the numerical calculations were performed on a CDC-6600 computer.

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CHAPTER I

INTRODUCTION

Since the prediction of the existence of the anti-electron by Dirac[4] and the subsequent discovery of the positron by Anderson[5] in 1932, the positron has been studied in various branches of physics. The first interest was to study its fundamental properties. Later, it has been used as a probe in problems of solid state and atomic physics. It is important to use as many different examples as possible in applying various approximations and methods developed in the theory of atomic collisions. Because of its positive charge, a positron is repelled by the mean static field of a neutral atom. Because a positron is not identical with a bound atomic electron there is no exchange to consider. Yet, a positron of suitably large energy can pick up an atomic electron to form a bound pair, the positronium atom, which recedes to infinity. If the captured electron has an opposite spin to the positron, forming para-positronium, the lifetime towards mutual annihilation is about 10^{-10} sec., but if the spins are parallel, forming ortho-positronium, the lifetime is about 10^{-7} sec. These lifetimes are long compared with the collision time which is of the order of 10^{-17} sec. Thus it is meaningful to talk about positronium formation by collision.

Being different from electron scattering by atoms, scattering of positrons by atoms serves as an interesting and distinct testing ground for atomic collision theory. The scattering of positrons by hydrogen atoms is one of the simplest cases to study theoretically. It has been studied extensively since the first work on the problem in 1954 by Massey and Mohr[6]. Very thorough and comprehensive accounts of the earlier work on the problem are given by Mott and Massey[7] and by several reviews by Burke and Smith[8], Fraser[9] and Bransden[10]. Only a few are discussed and mentioned here.

Spruch and Rosenberg[11] first obtained a negative upper bound for the scattering length, showing that at low energy, the positron experiences an attractive force from the target atom. Schwartz[12] in 1961 obtained variationally very accurate and reliable scattering length and S-wave phase shifts, using a trial wave function of 53 terms. Since then, the calculations on the problem have been done not necessarily with the aim to improve Schwartz' results, but to get close to his by taking different approximations, trying to reduce the work involved in the elaborate variational calculation.

Smith[13] in 1961 formulated the theory in which the wave function is expanded in a double sum of eigen states of both hydrogen and positronium. Cody, Lawson, Massey

and Smith[14] studied the importance of various physical effects one has to consider in this problem to improve the result. They considered the static approximation, in which the target atom is assumed to remain unchanged as the positron approaches, and the static+virtual positronium approximation, in which one takes into consideration the effect of positronium being formed in the scattering region as an intermediate stage of the elastic scattering. They also considered adding to the static field a polarization potential given by the Temkin-Lamkin[15] approximation (e.g. Mott and Massey[7]) which accounts for the physical effect that the hydrogen atom is polarized and exerts an attraction on the incoming positron. In the latter cases, the phase shifts are raised from the poor value of the static approximation but are still much lower than Schwartz' results. Further, Cody et al[14] have also considered adding the Temkin-Lamkin polarization potential on top of the static+virtual positronium approximation, and obtained results overshooting those of Schwartz, showing that taking virtual positronium and polarization effects together overestimates the attraction between the positron and the hydrogen atom.

An important advance in the problem came with the development of the bound principle due to the work of Hahn, O'Malley and Spruch[16-18], McKinley and Macek[19] and of Gailitis[20]. The importance of a formulation in which

the calculation gives a bound to the scattering parameters has repeatedly been stressed. It not only gives a meaningful result without relying on comparison with an experiment, but also can distinguish the better of two calculations both satisfying the bound principle; the calculation that gives a higher value is superior if it gives a lower bound.

McEachran and Fraser[21] in 1965 did a close coupling approximation using 6 hydrogenic states (1s-2s-2p-3s-3p-3d) in the expansion: their results not only demonstrated the bound principle, but also showed, unlike the electron-hydrogen case, the convergence in the hydrogen eigen-function expansion is very slow in the positron-hydrogen problem. Schwartz' results, though accurate and reliable, do not give a bound, while the close coupling approximation and the double eigen function expansion method of Smith[13] give a lower bound to the phase shifts. Hahn and Spruch[22] in 1965 obtained a lower bound to the S-wave phase shifts very close to but lower than those of Schwartz.

Drachman[23] has considered the effect of adding the adiabatic polarization potential of Dalgarno and Lynn[24] on top of the repulsive mean static field. The S-wave phase shifts obtained are higher than those of Schwartz by quite a margin. However, with an energy-independent parameter to suppress 90% of the short range part of the potential coming from the monopole component, he has managed to get good agreement with Schwartz' results. This mono-

pole suppression is empirical, and the formulation does not satisfy a bound principle. Later[25], he has used the adiabatic trial wave function in such a way that gives lower bounds to the phase shifts, and has obtained results somewhat lower than the more elaborate calculation of Hahn and Spruch[22].

Recently Bhatia et al[1] have done a calculation, similar to the work of Gailitis[26] on the electron-hydrogen problem, using up to 84 terms in approximating the closed channel part of the wave function, and obtained the most accurate lower bounds on the S-wave phase shifts to date. Their result will take the place of Schwartz' in serving as 'the solution' to the problem for energies up to the positronium formation threshold.

The Harris variational method[27] has been applied by Houston and Drachman[28] to give very good S-wave phase shifts in agreement with those of Ref.(1) to the third figure. A variant of the eigen function expansion method is the pseudo-state expansion, in which the higher bound and continuum states are represented by discrete states, orthogonal to the bound states and to each other. It has been shown to increase convergence in the electron-hydrogen problem (Damburg and Geltman[29], and Burke, Gallaher and Geltman[30]). Such an expansion has been applied to the positron-hydrogen problem recently by Fon and Gallaher[31], who solve for the scattering function variationally and preserve the bound property of the close coupling approx-

imation. Their 3-state (1s-2s-$2\bar{p}$) results show some improvement over the 6-hydrogenic-state expansion of McEachran and Fraser[21], but are still considerably lower than the accurate results of Bhatia et al[1].

A double eigen function expansion with different numbers of states, including pseudo-states, has been carried out by Wakid and LaBahn[32]. They use the Nesbet algebraic expansion method[33,34] to solve for the scattering function; in doing so, the bound on the phase shifts and R-matrix is lost. Their phase shifts from the expansion (H(1s)-H($\overline{2p}$)-Ps(1s)-Ps($\overline{2p}$)) show some improvement over the results of Fon and Gallaher, but are still not satisfactory when compared with the results of Ref.(1), showing that convergence in the pseudo-state expansion is still slow in the positron-hydrogen problem.

Works on positronium formation by positrons colliding with hydrogen atoms are not as numerous as on elastic scattering. Earlier work includes the Born approximation of Massey and Mohr[6] and the impulse approximation of Cheshire[35]. Bransden and Jundi[36] have extended their earlier work[37] to this energy region and obtained formation cross-sections in the two-state approximation. They also have considered the effects of adding various multipoles of the polarization potential in each of the hydrogen and positronium channel. Similar calculations have also been performed by Fels and Mittleman[38].

Since both the hydrogen and positronium state functions are known exactly, the positron-hydrogen system is an ideal case with which to study rearrangement collisions. The non-orthogonality of the hydrogen and positronium states complicates the projection operator formulation[39] in this energy region. Based on an earlier generalised variational bound formulation by Hahn[40], Dirks and Hahn[41] recently have obtained a lower bound on the L=0 R-matrix. The truncated eigen function expansion + short range correlations formulation of Gailitis[20] is mathematically equivalent to the formulation by Hahn et al[16-18] in providing a bound principle, and is easier to apply in practice. This fact and the important observation by Burke and Taylor[42] that the correlation terms need not be orthogonal to the open channel part of the wave function give the start of this thesis work.

Mittleman[2] in 1966 has shown that for positron-hydrogen scattering, similar to the electron-hydrogen case, an infinite series of resonances may exist below the excitation thresholds for both hydrgen and positronium atoms. The physical basis for this phenomenon arises from the degeneracy of the excited states giving rise to very long range attractive forces. A resonance will show up in a scattering calculation in which the phase shift or the eigen phase rises sharply through π in a very narrow energy range. It can also be found by solving an eigen-

value problem for a modified Hamiltonian in which the open channel part is projected out.

A scattering calculation, by Seiler et al[43], using the algebraic close coupling method, with three hydrogenic states in the expansion produces three of such resonances for the S-wave at energies close to the n=2 excitation threshold of hydrogen. Since the positronium channel is completely neglected in their calculation, these resonances may or may not persist in the real problem; they may well be shifted to higher energies. From the Q-operator formalism of Feshbach[39], a resonance can be looked upon approximately as a bound state[44]. Hahn and Dirks[45] use this approach to find such resonances, but with a negative result in the S-wave. From their calculation, they conclude that either there are no resonances below the excitation threshold for hydrogen or they are very close to the threshold.

It is worth mentioning that the three particles, a positron, an electron and a proton, cannot form a bound state[46] unless the positron has a hypothetical mass m_p greater than $2.2m_e$[47], and that there is no resonant state below the positronium formation threshold[1,48].

Unfortunately, up to the present, there is no experimental report on the problem. One reason is that it is difficult to obtain a monoergic beam of low energy positrons with sufficient intensity to do a collision

experiment. Further, the conventional positron swarm experiments, carried out by many on noble gases, are not readily practicable for the case of hydrogen atoms.

CHAPTER II

THEORY AND FORMALISM

The Schrodinger Equation

The Schrodinger Equation describing the system of an electron and a positron moving with respect to the proton which is taken to be infinitely massive and fixed at the origin of the coordinate system is

$$\left(-\frac{\hbar^2}{2m}\nabla_r^2 - \frac{\hbar^2}{2m}\nabla_p^2 - \frac{e^2}{r} + \frac{e^2}{r_p} - \frac{e^2}{|\bar{r}-\bar{r}_p|} - E\right)\Psi(\bar{r},\bar{r}_p) = 0 \quad (2.1)$$

where $\bar{r}$ denotes the position vector of the electron and $\bar{r}_p$ that of the positron with respect to the proton. Since the total angular momentum is conserved during the collision process , and we neglect spin-dependent forces, we can work on a state with orbital angular momentum L=0. Generalization to higher orbital angular momentum states is straightforward.

In order to suppress some of the constant factors involving $\hbar$, e and m etc., we use atomic units in which $\hbar$=1, m=½ and e^2=2. The unit of length is the Bohr radius of the hydrogen atom, $a_o=\hbar^2/(me^2)=0.53\times10^{-8}$cm. and the unit of energy is the Rydberg $=e^2/2a_o=13.6$eV. Cross-sections are given in $\pi a_o^2=8.8\times10^{-17}cm^2$.

We picture a positron with momentum $\bar{k}$, and therefore

kinetic energy k^2 , colliding with a hydrogen atom in its ground state with energy -1; the total energy of the system is $E=-1+k^2$. We have the folowing reactions

$$\begin{aligned} e^+ + H(1s) &\rightarrow e^+ + H(1s) \\ &\rightarrow Ps(1s) + H^+ \\ &\rightarrow e^+ + H^* \\ &\vdots \end{aligned}$$

Each reaction, denoting a final outcome of the scattering process, constitutes a 'channel'. Not all reactions are possible. If a reaction is energetically possible, we say that the channel corresponding to that reaction is open, otherwise it is closed.

A positronium atom with its mass being $M = 2m$, and momentum $\bar{\kappa}$, has kinetic energy $\frac{1}{2}\kappa^2$. Therefore we have the relation $E=k^2-1=\frac{1}{2}\kappa^2-\frac{1}{2}$ (the binding energy of ground state positronium is $\frac{1}{2}$). For all positive energies k^2 of the incoming positron, the first, or the elastic, channel is always open. For the second channel to be open, we must have $\frac{1}{2}\kappa^2 \geq 0$, or $E \geq -\frac{1}{2}$; similarly for the third channel open, $E \geq -\frac{1}{4}$, and so on. The number of channels open will increase rapidly with energy. We limit ourselves to $E<-\frac{1}{4}$, so that we have at most two channels, the elastic channel and the positronium formation channel, open.

The R-Matrix and Cross Section Formulas

In atomic units, the Schrodinger Equation (2.1) is written as

$$(-\nabla_r^2 - \nabla_p^2 - \frac{2}{r} - \frac{2}{|\bar{r}-\bar{r}_p|} + \frac{2}{r_p} + 1-k^2)\Psi(\bar{r},\bar{r}_p) = 0 \qquad (2.2)$$

with Ψ behaving asymptotically as

$$\Psi \underset{\substack{r \text{ finite} \\ r_p \to \infty}}{\sim} \psi(r)F(r_p)$$

$$\underset{\substack{\rho \text{ finite} \\ \sigma \to \infty}}{\sim} \phi(\rho)G(\sigma) \qquad (2.3)$$

where $\bar{\rho} = \bar{r}-\bar{r}_p$ and $\bar{\sigma} = (\bar{r}+\bar{r}_p)/2$ are the internal and centre of mass coordinates of the positronium atom. $\psi(r)$ and $\phi(\rho)$ are the ground state wave functions of hydrogen and positronium. They satisfy the equations

$$\begin{aligned} &(-\nabla_r^2 - \frac{2}{r} + 1)\psi(r) = 0 \\ &(-2\nabla_\rho^2 - \frac{2}{\rho} + \tfrac{1}{2})\phi(\rho) = 0 \end{aligned} \qquad (2.4)$$

and are explicitly given by

$$\psi(r) = (1/\sqrt{\pi})\exp(-r)$$

and $\qquad (2.5)$

$$\phi(\rho) = (1/\sqrt{8\pi})\exp(-\rho/2).$$

The functions $F(r_p)$ and $G(\sigma)$ satisfy asymptotically the free particle equations

$$(\nabla_p^2 + k^2) F(r_p) = 0$$

and (2.6)

$$(\tfrac{1}{2}\nabla_\sigma^2 + \tfrac{1}{2}\kappa^2) G(\sigma) = 0.$$

We denote two linearly independent solutions of (2.2) by Ψ_ν, $\nu=1,2$. Since F and G satisfy asymptotically (2.6), we require F and G to take the real asymptotic forms

$$\begin{aligned}
F_1(r_p) &\underset{r_p \to \infty}{\sim} \frac{1}{r_p}\sqrt{(\frac{m}{k})}\{\sin(kr_p) + R_{11}\cos(kr_p)\} \\
G_1(\sigma) &\underset{\sigma \to \infty}{\sim} \frac{1}{\sigma}\sqrt{(\frac{M}{\kappa})}R_{21}\cos(\kappa\sigma) \\
F_2(r_p) &\underset{r_p \to \infty}{\sim} \frac{1}{r_p}\sqrt{(\frac{m}{k})}R_{12}\cos(kr_p) \\
G_2(\sigma) &\underset{\sigma \to \infty}{\sim} \frac{1}{\sigma}\sqrt{(\frac{M}{\kappa})}\{\sin(\kappa\sigma) + R_{22}\cos(\kappa\sigma)\}
\end{aligned} \qquad (2.7)$$

in terms of the symmetric reactance- or the R-matrix*. Here it is a 2x2 matrix for we have two channels open. It is related to the S- and T-Matrix by the relations[49]

$$T = \frac{-2iR}{1-iR}$$

and

$$S = 1-T.$$

The R-Matrix may be diagonalized by an orthogonal matrix U

---

* It is also known as the K-Matrix.

as

$$URU^{-1} = \begin{pmatrix} \tan \delta_1 & 0 \\ 0 & \tan \delta_2 \end{pmatrix} \tag{2.8}$$

(see e.g. Mott and Massey, pp.371-372), where δ_1 and δ_2 are the eigen phases. The S-wave contribution to the cross section for the reaction from channel ν to ν' is given by

$$\sigma_{\nu\nu'} = \frac{4}{k_\nu^2} \left| \left(\frac{R}{1-iR}\right)_{\nu\nu'} \right|^2 \tag{2.9}$$

in units of πa_o^2, with $k_1 = k$ and $k_2 = \kappa$.

In the case of $E < -\frac{1}{2}$, $\kappa^2 < 0$, we have only one channel open. Asymptotically we have, where α is a constant,

$$\begin{aligned} F(r_p) &\underset{r_p \to \infty}{\sim} \frac{1}{r_p} \sqrt{\left(\frac{m}{k}\right)} \{\sin(kr_p) + \tan\eta_0 \cos(kr_p)\} \\ G(\sigma) &\underset{\sigma \to \infty}{\sim} \frac{1}{\sigma} \alpha \exp(-\kappa\sigma). \end{aligned} \tag{2.10}$$

The R-matrix has only one element, $R_{11} = \tan \eta_0$, the tangent of the phase shift η_0. The $L=0$ contribution to the total elastic scattering cross section is then given by

$$\sigma_{11} = \frac{4}{k^2} \sin^2\eta_0. \tag{2.11}$$

Variational Principle

Let ψ_ν and $\psi_{\nu'}$ denote two solutions of (2.2) having

the asymptotic forms (2.7). We form the functional

$$I_{\nu\nu'} = \langle \Psi_\nu | H-E | \Psi_{\nu'} \rangle \ .$$

If Ψ_ν varies about the exact value by $\delta\Psi_\nu$ such that Ψ_ν asymptotically varies from the form (2.7) by

$$\delta\Psi_\nu \underset{r_p \to \infty}{\sim} \psi(r)\frac{1}{r_p}\sqrt{\left(\frac{m}{k}\right)}\ \delta R_{1\nu}\cos(kr_p)$$

$$\underset{\sigma \to \infty}{\sim} \phi(\rho)\frac{1}{\sigma}\sqrt{\left(\frac{M}{\kappa}\right)}\ \delta R_{2\nu}\cos(\kappa\sigma) \ ,$$

the Kohn variational principle[50] may be written as

$$\delta(I - R)_{\nu\nu'} = 0 \ . \tag{2.12}$$

Let us take a trial wave function

$$\Psi^t(\bar{r},\bar{r}_p) = \psi(r)F^t(r_p)+\phi(\rho)G^t(\sigma)+\sum_{j=1}^{n} c_j\theta_j(\bar{r},\bar{r}_p) \tag{2.13}$$

with

$$\begin{aligned} r_p F^t(r_p) &\underset{r_p \to 0}{\sim} 0 \\ \sigma\, G^t(\sigma) &\underset{\sigma \to 0}{\sim} 0 \end{aligned} \tag{2.14}$$

and

$$\begin{aligned} F_1^t(r_p) &\underset{r_p \to \infty}{\sim} \frac{1}{r_p}\sqrt{\left(\frac{m}{k}\right)}\ \{\sin(kr_p)+R_{11}^t\cos(kr_p)\} \\ G_1^t(\sigma) &\underset{\sigma \to \infty}{\sim} \frac{1}{\sigma}\sqrt{\left(\frac{M}{\kappa}\right)}\ R_{21}^t\cos(\kappa\sigma) \end{aligned} \tag{2.15}$$

$$F_2^t(r_p) \underset{r_p \to \infty}{\sim} \frac{1}{r_p}\sqrt{\frac{m}{k}}\, R_{12}^t \cos(kr_p)$$

$$G_2^t(\sigma) \underset{\sigma \to \infty}{\sim} \frac{1}{\sigma}\sqrt{\frac{M}{\kappa}}\, \{\sin(\kappa\sigma) + R_{22}^t \cos(\kappa\sigma)\} \quad .$$

θ_j are some prescribed square-integrable functions such that $\bar{L}\theta_j = 0$, where $\bar{L}$ is the total orbital angular momentum operator. The unknown functions F^t, G^t and constants c_j are to be determined.

Similarly we can form the functional

$$I_{\nu\nu'}^t = \langle \Psi_\nu^t | H-E | \Psi_{\nu'}^t \rangle \quad .$$

By requiring the trial wave function Ψ_ν^t to possess the property (2.12) of the exact solution,

$$\delta(I^t - R^t)_{\nu\nu'} = 0, \tag{2.16}$$

where in (2.16) the variations are to be taken about F^t, G^t, and c_j such that

$$r_p \delta F_\nu^t(r_p) \underset{r_p \to 0}{\sim} 0$$

$$\sigma \delta G_\nu^t(\sigma) \underset{\sigma \to 0}{\sim} 0$$

and

$$\delta F_\nu^t(r_p) \underset{r_p \to \infty}{\sim} \frac{1}{r_p}\sqrt{\frac{m}{k}}\, \delta R_{1\nu}^t \cos(kr_p)$$

$$\delta G_\nu^t(\sigma) \underset{\sigma \to \infty}{\sim} \frac{1}{\sigma}\sqrt{\frac{M}{\kappa}}\, \delta R_{2\nu}^t \cos(\kappa\sigma) \quad , \tag{2.18}$$

the following coupled equations for F^t, G^t and c_j are obtained:

$$\langle\psi|H-E|\psi F^t + \phi G^t + \sum_j c_j\theta_j\rangle = 0 \quad * \qquad (2.19a)$$

$$\langle\phi|H-E|\psi F^t + \phi G^t + \sum_j c_j\theta_j\rangle = 0 \qquad (2.19b)$$

$$\langle\theta_i|H-E|\psi F^t + \phi G^t + \sum_j c_j\theta_j\rangle = 0 \; . \qquad (2.19c)$$

The solutions of (2.19) give approximate values R^t, for the R-matrix elements. To estimate the 'error' in R, we write $\Delta\Psi_\nu = \Psi_\nu^t - \Psi_\nu$ and $\Delta R_{\nu\nu'} = R^t_{\nu\nu'} - R_{\nu\nu'}$ as the errors in Ψ_ν and $R_{\nu\nu'}$. From (2.12) we have

$$R^t_{\nu\nu'} - R_{\nu\nu'} = \Delta I_{\nu\nu'}$$

$$= I^t_{\nu\nu'} - \langle\Delta\Psi_\nu|H-E|\Delta\Psi_{\nu'}\rangle .$$

Using Ψ^t of the form (2.13) and from (2.19) it can be shown that $I^t_{\nu\nu'} = 0$. The error in the calculated R-matrix elements $R^t_{\nu\nu'}$ is thus of second order in the error in the wave function. Further, it will be proved later that $\Delta R_{\nu\nu}$ are negative up to a certain energy and $R^t_{\nu\nu}$ are lower bounds to $R_{\nu\nu}$.

The Coupled Equations

After some manipulations, equations (2.19) are simplified to

$$(\nabla_p^2+k^2)F^t(r_p) = U(r_p)F^t(r_p) + \int d\bar{\sigma}\, K_{12}^{cs}(\bar{r}_p,\bar{\sigma})G(\sigma) + \sum_j c_j V_j(r_p) \qquad (2.20a)$$

*Here it is understood that the integration is taken over the variable common to the ket and bra.

$$\frac{1}{2}(\nabla_\sigma^2+\kappa^2)G^t(\sigma) = \int d\bar{r}_p\ K_{21}^{cs}(\bar{r}_p,\bar{\sigma})F^t(r_p) + \sum_j c_j W_j(\sigma) \quad (2.20b)$$

$$\sum_j (EN_{ij}-H_{ij})c_j = \int d\bar{r}_p\ V_i(r_p)F^t(r_p) + \int d\bar{\sigma}\ W_i(\sigma)G^t(\sigma) \quad (2.20c)$$

where $U(r_p) = \langle\psi|2/r_p-2/\rho|\psi\rangle = 2(1+1/r_p)\exp(-2r_p)$ is the 'static field' of the hydrogen atom felt by the positron,

$$K_{12}^{cs}(\bar{r}_p,\bar{\sigma}) = 8(-\tfrac{1}{2}\nabla_\sigma^2 - \frac{2}{|2\bar{\sigma}-\bar{r}_p|} + \frac{2}{r_p} + \tfrac{1}{2}k^2)\psi(|2\bar{\sigma}-\bar{r}_p|)\phi(|2\bar{\sigma}-2\bar{r}_p|) \quad (2.21a)$$

$$K_{21}^{cs}(\bar{r}_p,\bar{\sigma}) = 8(-\nabla_p^2+\frac{2}{r_p} - \frac{2}{|2\bar{\sigma}-2\bar{r}_p|} - k^2)\psi(|2\bar{\sigma}-\bar{r}_p|)\phi(|2\bar{\sigma}-2\bar{r}_p|) \quad (2.21b)$$

are the kernels resulting from the 'coupled static' approximation, in which all the c_j in the trial wave function (2.13) are put to zero, and

$$V_j(r_p) = \langle\psi|H-E|\theta_j\rangle \quad (2.21c)$$

$$W_j(\sigma) = \langle\phi|H-E|\theta_j\rangle \quad (2.21d)$$

$$H_{ij} = \langle\theta_i|H|\theta_j\rangle \quad (2.21e)$$

$$N_{ij} = \langle\theta_i|\theta_j\rangle \quad . \quad (2.21f)$$

The system (2.20) can further be simplified by eliminating c_j from (2.20a) and (2.20b). First we find the eigenvalues ε^λ and eigen vectors a_j^λ of the eigenvalue problem

$$\sum_{j=1}^{n} (H_{ij} - \varepsilon^\lambda N_{ij})\ a_j^\lambda = 0. \quad (2.22)$$

Then we write the last term of the sum in (2.13) as

$$\sum_{j=1}^{n} c_j \theta_j(\bar{r},\bar{r}_p) = \sum_{\lambda=1}^{n} b^\lambda \chi^\lambda(\bar{r},\bar{r}_p)$$

where the $\chi^\lambda(\bar{r},\bar{r}_p)$ are given by

$$\chi^\lambda = \sum_{j=1}^{n} a_j^\lambda \theta_j$$

We see that χ^λ form an orthonormal set with respect to which the Hamiltonian H of the system is diagonal. The c_j and b^λ are related by

$$c_j = \sum_{\lambda=1}^{n} a_j^\lambda b^\lambda \ . \qquad (2.23)$$

With the notation

$$V^\lambda(r_p) = \langle\chi^\lambda|H-E|\psi\rangle = \Sigma\ a_j^\lambda V_j(r_p)$$

$$W^\lambda(\sigma) = \langle\chi^\lambda|H-E|\phi\rangle = \Sigma\ a_j^\lambda W_j(\sigma) \ ,$$

b^λ can be obtained from (2.20c) as

$$b^\lambda = \frac{1}{(E-\varepsilon^\lambda)} \left(\langle V^\lambda|F^t\rangle + \langle W^\lambda|G^t\rangle\right) \ . \qquad (2.24)$$

The relation

$$\sum_{i,j} a_i^\lambda N_{ij} a_j^\mu = \delta_{\lambda\mu}$$

and (2.22) have been used in obtaining the last equation. Substituting this into the first two equations of (2.20),

we get

$$(\nabla_p^2+k^2)F^t(r_p) = U(r_p)F^t(r_p) + \int d\bar{\sigma}' K_{12}^{cs}(\bar{r}_p,\bar{\sigma}')G^t(\sigma') + \sum_\lambda \frac{V^\lambda(r_p)}{(E-\varepsilon^\lambda)}\left(\int d\bar{r}_p' V^\lambda(r_p')F^t(r_p') + \int d\bar{\sigma}' W^\lambda(\sigma')G^t(\sigma')\right) \quad (2.25a)$$

and

$$\tfrac{1}{2}(\nabla_\sigma^2 + \kappa^2)G^t(\sigma) = \int d\bar{r}_p' K_{21}^{cs}(\bar{r}_p',\bar{\sigma})F^t(\bar{r}_p') + \sum_\lambda \frac{W^\lambda(\sigma)}{(E-\varepsilon^\lambda)}\left(\int d\bar{r}_p' V^\lambda(r_p')F^t(r_p') + \int d\bar{\sigma}' W^\lambda(\sigma')G^t(\sigma')\right) \quad (2.25b)$$

The Radial Equations

Since we are taking Ψ to be a state of angular momentum $L = 0$, we define the radial functions $f^t(r_p)$ and $g^t(\sigma)$ by

$$F^t(r_p) = \frac{f^t(r_p)}{r_p} \qquad \text{and} \qquad G^t(\sigma) = \frac{g^t(\sigma)}{\sigma}. \quad (2.26)$$

From now on the superscript t will be dropped. After performing all the angular integrations, we have the following coupled integro-differential equations for $f(r_p)$ and $g(\sigma)$:

$$\left(\frac{d^2}{dr_p^2} + k^2\right) f(r_p) = U(r_p) f(r_p) + \int_0^\infty dr_p' \, \mathcal{K}_{11}(r_p, r_p') f(r_p') + \int_0^\infty d\sigma' \, \mathcal{K}_{12}(r_p, \sigma') g(\sigma') \tag{2.27a}$$

$$\left(\frac{d^2}{d\sigma^2} + \kappa^2\right) g(\sigma) = 2\int_0^\infty dr_p' \, \mathcal{K}_{21}(r_p', \sigma) f(r_p') + 2\int_0^\infty d\sigma' \, \mathcal{K}_{22}(\sigma, \sigma') g(\sigma') \tag{2.27b}$$

where

$$\mathcal{V}^\lambda(r_p) = \sqrt{4\pi}\, r_p V^\lambda(r_p) \tag{2.28a}$$

$$\mathcal{W}^\lambda(\sigma) = \sqrt{4\pi}\, \sigma\, W^\lambda(\sigma) \tag{2.28b}$$

$$\mathcal{K}_{12}^{cs}(r_p, \sigma) = \frac{r_p \sigma}{4\pi} \int\int d\hat{r}_p d\hat{\sigma}\; K_{12}^{cs}(\bar{r}_p, \bar{\sigma}) \tag{2.28c}$$

$$\mathcal{K}_{21}^{cs}(r_p, \sigma) = \frac{r_p \sigma}{4\pi} \int\int d\hat{r}_p d\hat{\sigma}\; K_{21}^{cs}(\bar{r}_p, \bar{\sigma}) \tag{2.28d}$$

$$\mathcal{K}_{11}(r_p, r_p') = \sum_\lambda \frac{\mathcal{V}^\lambda(r_p)\, \mathcal{V}^\lambda(r_p')}{E - \varepsilon^\lambda} \tag{2.28e}$$

$$\mathcal{K}_{12}(r_p, \sigma) = \mathcal{K}_{12}^{cs}(r_p, \sigma) + \sum_\lambda \frac{\mathcal{W}^\lambda(\sigma)\, \mathcal{V}^\lambda(r_p)}{E - \varepsilon^\lambda} \tag{2.28f}$$

$$\mathcal{K}_{21}(r_p, \sigma) = \mathcal{K}_{21}^{cs}(r_p, \sigma) + \sum_\lambda \frac{\mathcal{V}^\lambda(r_p)\, \mathcal{W}^\lambda(\sigma)}{E - \varepsilon^\lambda} \tag{2.28g}$$

and

$$\mathcal{K}_{22}(\sigma, \sigma') = \sum_\lambda \frac{\mathcal{W}^\lambda(\sigma)\, \mathcal{W}^\lambda(\sigma')}{E - \varepsilon^\lambda} \quad . \tag{2.28h}$$

The boundary conditions are, from (2.14) and (2.15)

$$f_\nu(0) = g_\nu(0) = 0 \tag{2.29}$$

$$f_\nu(r_p) \underset{r_p \to \infty}{\sim} \sqrt{(\frac{m}{k})}\{\delta_{1\nu} \sin(kr_p) + R_{1\nu} \cos(kr_p)\} \tag{2.30a}$$

$$g_\nu(\sigma) \underset{\sigma \to \infty}{\sim} \sqrt{(\frac{M}{\kappa})}\{\delta_{2\nu} \sin(\kappa\sigma) + R_{2\nu} \cos(\kappa\sigma)\} . \tag{2.30b}$$

The kernels K_{12}^{cs} and K_{21}^{cs} can be shown to be equal (see Appendix A). Thus from (2.28f) and (2.28g) $\mathcal{K}_{12}$ and $\mathcal{K}_{21}$ are equal also. Nevertheless the coupled equations (2.27) are not quite symmetric; there is a factor of 2 in the second equation. It comes from the fact that the channel masses are different, the positronium mass is twice that of the positron. Equations (2.27) with (2.28-2.30) are the equations solved in this work.

The Minimum Principle

We follow closely the work of Gailitis[20] in establishing the minimum or bound principle. First we prove the monotonicity theorem on the R-matrix. Let us consider the Schrodinger Equation for S-wave scattering

$$\tilde{L}\tilde{F} \equiv \{\frac{1}{\tilde{m}} (\frac{\tilde{d}^2}{dr^2} + \tilde{k}^2) - \tilde{V}\}\tilde{F} = 0 \tag{2.31}$$

with the boundary condition at infinity

$$\tilde{F} \sim \sqrt{\left(\frac{\tilde{m}}{\tilde{k}}\right)} (\sin \tilde{\rho} + \cos \tilde{\rho}\ R) \qquad (2.32)$$

$$\tilde{\rho} = \tilde{k}\tilde{r} \ .$$

$\tilde{F}$ is a square matrix whose columns are different linearly independent solutions of (2.31); $\tilde{m}$, $\tilde{k}$ are diagonal matrices whose elements are respectively the reduced masses and the wave numbers of the channels. Let us consider two such equations with potentials $\tilde{V}_1$ and $\tilde{V}_2$, and solutions $\tilde{F}_1$ and $\tilde{F}_2$. We form the matrix

$$\int_0^\infty (\tilde{F}_2^T \tilde{L}_1 \tilde{F}_1 - \tilde{F}_1^T \tilde{L}_2 \tilde{F}_2) d\tilde{r} = 0 \ . \qquad (2.33)$$

On integrating by parts, using the properties that $\tilde{V}$ be self-adjoint and R symmetric and adding to the resulting equation its transpose, we have

$$R_2 - R_1 = \frac{1}{2} \int_0^\infty \{\tilde{F}_1^T (\tilde{V}_1 - \tilde{V}_2) \tilde{F}_2 + \tilde{F}_2^T (\tilde{V}_1 - \tilde{V}_2) \tilde{F}_1\} d\tilde{r} \ . \qquad (2.34)$$

Therefore we see that if $\tilde{V}$ varies by a small quantity $\delta\tilde{V}$ and at the same time R varies by δR, then

$$\delta R = - \int_0^\infty \tilde{F}^T \delta\tilde{V} \tilde{F}\ d\tilde{r} \ . \qquad (2.35)$$

If $\tilde{V}_1 \geq \tilde{V}_2$ and the matrix R varies continuously from R_1 to R_2, then $R_2 \geq R_1$. Here $R_2 \geq R_1$ means $(R_2 - R_1)$ is positive definite; it follows that $R^2_{\nu\nu} \geq R^1_{\nu\nu}$, but for $\nu \neq \nu'$, $R^2_{\nu\nu'} \geq R^1_{\nu\nu'}$ is not necessarily true. In the case of one

open channel, R has only one element, $\tan \eta_o$. If the potential is made more negative, $\tan \eta_o$ will increase.

Next, we follow the projection operator formalism of Feshbach[39]. We define a projection operator P such that it projects onto the open channel part of ψ. We also define a Q by $Q = 1 - P$. We can write the Schrodinger Equation as

$$P(H-E)(P+Q)\Psi = 0$$

$$Q(H-E)(P+Q)\Psi = 0 \ ,$$

leading to

$$P(H-E)P\Psi = -PHQ\psi$$

$$Q(H-E)Q\Psi = -QHP\psi \quad . \tag{2.36}$$

Dropping $Q\Psi$ in the first of (2.36), we get

$$P(H-E)P\Psi = 0 \tag{2.37}$$

which is often used as a scattering approximation. Eliminating $Q\Psi$ from the second of (2.36) we have the exact equation

$$P(H - E + HQ \frac{1}{Q(E - H)Q} QH)P\Psi = 0 \tag{2.38}$$

which is different from (2.37) by the addition of the optical potential V_{opt} ,

$$V_{opt} = PHQ \frac{1}{Q(E - H)Q} QHP \tag{2.39}$$

If E is less than the lowest eigen value of the operator QHQ, then V_{opt} is negative. From the monotonicity theorem, the R-matrix obtained from (2.37) would be lower than the true R from (2.38). Equation (2.38) may be cast into the

form of (2.31), the starting point of Gailitis' demonstration.

Because of the non-orthogonality of the ground state wave functions of hydrogen and positronium, it is difficult to write down a simple P such that $P\Psi$ has the property (2.3) of Ψ at asymptotic region. The form given by Chen and Mittleman[51], which uses the positron coordinate rather than that of the centre of mass, to label positronium, is difficult to apply. Hahn[52] has found a way to get around this by writing the Schrodinger Equation as a two component matrix equation

$$(\tilde{H} - \tilde{E})\tilde{\Psi} = \begin{pmatrix} H-E & H-E \\ H-E & H-E \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = 0 \ .$$

Each component of $\tilde{\Psi} = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}$ is associated with each open channel configuration of the system. One can define a $\tilde{P}$ and $\tilde{Q}$ by

$$\tilde{P} = \begin{pmatrix} P_1 & 0 \\ 0 & P_2 \end{pmatrix} \qquad \text{and} \qquad \tilde{Q} = 1 - \tilde{P} \tag{2.40}$$

with $P_1 = |\psi><\psi|$ and $P_2 = |\phi><\phi|$, so that we have

$$\tilde{P}\,\tilde{\Psi} \sim \begin{pmatrix} \psi F \\ \phi G \end{pmatrix}$$

By writing $\tilde{\Psi} = \tilde{P}\tilde{\Psi} + \tilde{Q}\tilde{\Psi}$, and multiplying from the left by $\tilde{P}$ and by $\tilde{Q}$, we get

$$\tilde{P}(\tilde{H} - \tilde{E})\tilde{P}\tilde{\Psi} = -\tilde{P}\tilde{H}\tilde{Q}\tilde{\Psi} \tag{2.41a}$$

$$\tilde{Q}(\tilde{H} - \tilde{E})\tilde{Q}\tilde{\Psi} = -\tilde{Q}\tilde{H}\tilde{P}\tilde{\Psi} \tag{2.41b}$$

Dropping the closed channel part $\tilde{Q}\tilde{\Psi}$, (2.41a) becomes

$$\tilde{P}(\tilde{H} - \tilde{E})\tilde{P}\tilde{\Psi} = 0 \tag{2.42}$$

which is the same as (2.19) with all the $c_i=0$, that is the equation from the coupled static approximation. Substituting $\tilde{Q}\tilde{\Psi} = \frac{1}{\tilde{Q}(\tilde{E} - \tilde{H})\tilde{Q}} \tilde{Q}\tilde{H}\tilde{P}\tilde{\Psi}$ from (2.41b) into (2.41a) we get

$$\tilde{P}(\tilde{H} - \tilde{E} + \tilde{V}_{opt})\tilde{P}\tilde{\Psi} = 0 \tag{2.43}$$

with the optical potential

$$\tilde{V}_{opt} = \tilde{P}\tilde{H}\tilde{Q} \frac{1}{\tilde{Q}(\tilde{E} - \tilde{H})\tilde{Q}} \tilde{Q}\tilde{H}\tilde{P} \tag{2.44}$$

which is negative for E lower than the lowest eigenvalue, ε_o, of the operator $\tilde{Q}\tilde{H}\tilde{Q}$.

Equation (2.43) is exact. We now try to approximate the Q part of Ψ. For a given set $\{\theta_i\}$ of n linearly independent square integrable functions, one can arbitrarily partition them into two subsets $\{\theta_\mu^{(1)}\}$ and $\{\theta_\nu^{(2)}\}$ of ℓ and m members respectively, with $\ell + m = n$.

Let $\Lambda_\mu^{(1)} = Q_1\theta_\mu^{(1)}$ and $\Lambda_\nu^{(2)} = Q_2\theta_\nu^{(2)}$

Now we introduce a projection operator $\tilde{A}$ such that it projects onto the entire two dimensional function space functions of the form

$$\tilde{A}\tilde{\Psi} = \begin{pmatrix} \psi F + \sum_{\mu=1}^{\ell} c_\mu^{(1)} \Lambda_\mu^{(1)} \\ \phi G + \sum_{\nu=1}^{m} c_\nu^{(2)} \Lambda_\nu^{(2)} \end{pmatrix} \tag{2.45}$$

with different functions F, G and coefficients $c_\mu^{(1)}$ and $c_\nu^{(2)}$.

One notes that $\tilde{A}\tilde{P} = \tilde{P}\tilde{A} = \tilde{P}$,

and $\tilde{Q}\tilde{A} = \tilde{A}\tilde{Q}$. (2.46)

We require our trial wave function $\tilde{\Psi}_t$ to satisfy

$$\tilde{A}(\tilde{H} - \tilde{E})\tilde{A}\tilde{\Psi}_t = 0 \tag{2.47}$$

which leads to

$$\tilde{A}(\tilde{H} - \tilde{E})\tilde{P}\tilde{A}\tilde{\Psi}_t + \tilde{A}(\tilde{H} - \tilde{E})\tilde{Q}\tilde{A}\tilde{\Psi}_t = 0$$

Operate on left by $\tilde{P}$ and by $\tilde{Q}$ and making use of (2.46), we get

$$\tilde{P}(\tilde{H} - \tilde{E})\tilde{P}\tilde{\Psi}_t = -\tilde{P}\tilde{H}\tilde{Q}\tilde{A}\tilde{\Psi}_t$$

and $$\tilde{A}\tilde{Q}(\tilde{H} - \tilde{E})\tilde{Q}\tilde{A}\tilde{\Psi}_t = -\tilde{A}\tilde{Q}\tilde{H}\tilde{P}\tilde{\Psi}_t$$

Upon eliminating $\tilde{Q}\tilde{A}\tilde{\Psi}_t$, we have

$$\tilde{P}(\tilde{H} - \tilde{E} + \tilde{H}\tilde{Q}\tilde{A}\frac{1}{\tilde{A}\tilde{Q}(\tilde{E} - \tilde{H})\tilde{Q}\tilde{A}}\tilde{A}\tilde{Q}\tilde{H})\tilde{P}\tilde{\Psi}_t = 0 \tag{2.48}$$

which is different from equation (2.43) in that the optical potential is now approximated by

$$\tilde{V}^t_{opt} = \tilde{P}\tilde{H}\tilde{Q}\tilde{A}\frac{1}{\tilde{A}\tilde{Q}(\tilde{E} - \tilde{H})\tilde{Q}\tilde{A}}\tilde{A}\tilde{Q}\tilde{H}\tilde{P} \tag{2.49}$$

which is now tractable in terms of the θ_i functions. We now wish to investigate under what conditions $\tilde{V}^t_{opt} \geq \tilde{V}_{opt}$ holds so that we can establish the relation $\tilde{R}^t \leq \tilde{R}$.

By introducing B = 1 - A and M = Q(H-E)Q, from the operator identity (for proof, see Appendix B)

$$M^{-1} - A(AMA)^{-1}A = M^{-1}B(BM^{-1}B)^{-1}BM^{-1} \qquad (2.50)$$

we can see that the inequality $\tilde{V}^{t}_{opt} \geq \tilde{V}_{opt}$ is satisfied when $BM^{-1}B \geq 0$, or when $E \geq \varepsilon_o$, the lowest eigenvalue of QHQ.

Burke and Taylor[42] made a very important observation in that θ_i need not be made orthogonal to the open channel space and yet a bound on R can still be obtained. It is because any P-part of θ_i may be slid into the form ψF and ϕG, and the θ_i do not contribute to the total trial wave function asymptotically, and hence do not affect the asymptotic boundary conditions on F and G. Since F and G are arbitrary functions determined by the Kohn's variation principle, we arrive at the same equations for F and G with the same boundary conditions independent of whether the θ_i lie entirely in the Q-space or not so long as they go to zero asymptotically.

It can be shown (Appendix C) that (2.47) gives the same equation (2.19) for the functions F and G and coefficients c_i. Thus we have established that using trial function (2.13), a variational calculation (2.16) will give a lower bound on the R-matrix for energies up to the lowest eigenvalues of $\tilde{Q}\tilde{H}\tilde{Q}$.

CHAPTER III

POSITRON ANNIHILATION WITH THE HYDROGEN ATOM

A positron colliding with hydrogen atoms may annihilate with a bound electron to give, most likely, two photons. Since we are concerned with low energy positrons, the total energy of the annihilating pair is $2mc^2$ (c being the velocity of light), each photon will have an energy of $mc^2 = 0.51\text{MeV}$. The cross section for two-photon annihilation of a free positron and a free electron is given by the expression

$$q_2 = 4(c/v)r_o^2 \tag{3.1}$$

where v is the relative velocity of the positron and electron, r_o is the classical electron radius = $\alpha^2 a_o$ = $2.8\text{x}10^{-13}$ cm. (α=1/137 is the fine structure constant). This expression was first obtained by Dirac based on a perturbation theory in which the positron and electron are described by unperturbed plane waves. The rate of annihilation into two photons when a beam of positrons goes through a medium with n free electrons per unit volume is

$$\Lambda_2 = \tfrac{1}{4}\, q_2 nv. \tag{3.2}$$

The factor ¼ comes from the fact that the electrons are distributed randomly so that on the average ¼ of the electrons are in a singlet spin state relative to the positron. Only from the singlet spin state can the two

annihilate to give two photons. If the medium contains N atoms or molecules per unit volume, and each has Z electrons, then n = NZ. Therefore

$$\Lambda_2 = \tfrac{1}{4}\, q_2 NZv = \pi c r_o^2 NZ. \qquad (3.3)$$

Considering that the electrons are in fact not free, the above expression should be modified. One introduces a velocity dependent parameter $Z_{eff}(v)$ that gives the number of electrons per atom or molecule effective in annihilation. Since $\Lambda_2 = \frac{1}{4} q_2 N v Z_{eff}$, the annihilation cross section per atom or molecule is

$$q_2^A = \tfrac{1}{4} q_2 Z_{eff} = \pi (c/v) r_o^2 Z_{eff}(v). \qquad (3.4)$$

As the scattering cross section σ is of the order of a_o^2 , and the ratio of annihilation to scattering cross section, $q_2^A/\sigma \sim (r_o^2/a_o^2)(c/v) Z_{eff}$. Even at very low energy, say 10^{-3}eV, $q_2^A/\sigma \sim 10^{-3} Z_{eff}$, at higher energies the ratio would be even smaller. We can thus ignore annihilation during the process of scattering of positrons by a gaseous medium of low Z.

A positron and electron pair can also annihilate to give three photons when they are in a triplet spin state. Assuming them both being free, the cross section is given by[53]

$$q_3 = (\pi^2 - 9)\alpha q_2/\pi \ . \qquad (3.5)$$

For an unpolarized beam of positrons, passing through a medium of n free electrons per unit volume, the annihilation rate is

$$\Lambda_3 = (3/4) q_3 n v. \qquad (3.6)$$

Comparing (3.2) and (3.6), we see that $\Lambda_3/\Lambda_2 = 1/370$; so the contribution to the total decay rate due to 3-photon annihilation can be ignored.

Annihilation of a positron and an electron takes place when they are within a Compton wavelength $\lambda\!\!\!^{-}_c = \hbar/(mc)$ of each other. As $\lambda\!\!\!^{-}_c = \alpha a_o$, this can be considered a point for atomic problems. The probability of finding a positron at the place of an electron is $|\Psi(\bar{r},\bar{r})|^2$, where $\Psi(\bar{r},\bar{r}_p)$ is our solution to Eqn. (2.2) with a normalization corresponding to one positron per unit volume asymptotically. So from the definition of Z_{eff} as the effective number of electrons coinciding with the positron, it is then given by

$$Z_{eff} = \int d\bar{r} \; | \; \Psi(\bar{r},\bar{r}) |^2 \; . \qquad (3.7)$$

A quantum electrodynamic treatment gives the same expression for Z_{eff} (Ferrell[54], Wallace[55] and Drachman[56]).

Theoretical Calculation of Z_{eff} .

The wave function corresponding to unit flux at infinity has the asymptotic form

$$\Psi(\bar{r},\bar{r}_p) \sim \psi(r)(\exp(i\bar{k}.\bar{r}_p) + \beta \exp(ikr_p)/r_p). \qquad (3.8)$$

After a partial wave decomposition, the S-wave part of (3.8) is

$$\Psi \sim \psi(r)\ \exp(i\eta_0)\ \sin(kr_p + \eta_0)/(kr_p). \qquad (3.9)$$

The trial wave function Ψ^t of (2.13) which is a solution of the Schrodinger Equation (2.2) has an overall normalization arbitrary. For Ψ^t corresponding to (3.9) asymptotically, we must have

$$\Psi^t \sim \psi(r)\ \left(\frac{\cos\ \eta_0}{k}\right)\ f(r_p)/r_p$$

with $\qquad f \sim \sin(kr_p) + \tan\eta_0\ \cos(kr_p)$

Using (3.7), the S-wave contribution of Ψ to Z_{eff} is

$$Z_{eff} = \left(\frac{\cos\ \eta_0}{k}\right)^2 \int d\bar{r}\left|\psi(r)\frac{f(r)}{r} + \phi(0)\frac{g(r)}{r} + \sum_i c_i\theta_i(\bar{r},\bar{r})\right|^2$$

$$= 4\pi\left(\frac{\cos\ \eta_0}{k}\right)^2\Bigg[\int_0^\infty dr\psi^2(r)f^2(r) + \int_0^\infty dr\phi^2(0)g^2(r)$$

$$+ \sum_i c_i^2\int_0^\infty dr\ r^2\xi_i^2(r,r,0) + 2\phi(0)\int_0^\infty dr\psi(r)f(r)g(r)$$

$$+ 2\sum_i c_i\int_0^\infty dr\ r\psi(r)f(r)\xi_i(r,r,0)$$

$$+ 2\phi(0)\sum_i c_i\int_0^\infty dr\ rg(r)\xi_i(r,r,0)$$

$$+ 2\sum_{i>j} c_ic_j\int_0^\infty dr\ r^2\xi_i(r,r,0)\xi_j(r,r,0)\Bigg] \qquad (3.10)$$

where $\theta_i(\bar{r},\bar{r}_p) \equiv \xi_i(r,r_p,\hat{r}.\hat{r}_p)$,and f,g and c_i are solutions to (2.27) with $f(r) \sim (\sin(kr) + \tan\eta_0\cos(kr))$.

Z_{eff} furnishes another meeting place between theory and experiment. As the theoretical value of Z_{eff} comes from the internal region of the wave function, while the cross sections from the asymptotic region, the two are supplementary to each other in the comparison of theoretical calculation with experimental results.

Inelastic Region

Below the positronium formation threshold, the incoming positron has insufficient energy to pick up a bound electron to form positronium, the annihilation rate comes solely from the 'direct contact' of the positron with the electron in the scattering region. Above the pick-up threshod, real positronium could be formed. We then have two processes contributing to the annihilation rate, by 'direct contact' and by positronium formation. The latter process has 'infinite time to operate' and may contribute significantly. Fels and Mittleman[57] have found that annihilation from positronium formation dominates at energies above threshold. Thus it is meaningless to talk about Z_{eff} in this energy region; annihilation is proportional to the positronium formation cross section.

CHAPTER IV

MATHEMATICAL METHODS OF SOLUTION

Eigenvalue Problem and Preparation of the Kernels

A typical term in the correlation functions in our wave function (2.13) takes the form

$$\theta_i(\bar{r},\bar{r}_p) = r^{\alpha_i} r_p^{\beta_i} \rho^{\gamma_i} \exp(-\lambda_i r-\mu_i r_p) P_{\ell_i}(\hat{r}.\hat{r}_p) \quad (4.1)$$

where P_ℓ is a Legendre polynomial, $\alpha_i,\beta_i,\gamma_i$ and ℓ_i are non-negative integers consistent with $\gamma_i \geq 0$, $\alpha_i,\beta_i \geq \ell_i$. We proceed to evaluate the expressions in (2.28). The integrals

$$\mathcal{U}_i(r_p) = \sqrt{4\pi}\, r_p \int d\bar{r}\ \psi(r)(H-E)\theta_i(\bar{r},\bar{r}_p)$$

$$= 2\int d\bar{r}\ \exp(-r)\left(-\nabla_p^2 - \frac{2}{|r-r_p|} + \frac{2}{r_p} - k^2\right)\theta_i(\bar{r},\bar{r}_p)$$

and

$$N_{ij} = \int d\bar{r}d\bar{r}_p\ \theta_i(\bar{r},\bar{r}_p)\theta_j(\bar{r},\bar{r}_p)$$

are easily worked out analytically, while for the expressions

$$\mathcal{W}_i(\sigma) = \sqrt{4\pi}\sigma \int d\bar{\rho}\,\phi(\rho)(H-E)\theta_i$$

$$= \frac{1}{\sqrt{2}}\int d\bar{\rho}\ \exp\left(-\frac{\rho}{2}\right)\left(-\tfrac{1}{2}\nabla_\sigma^2 - \frac{2}{|\sigma+\frac{1}{2}\rho|} + \frac{2}{|\sigma-\frac{1}{2}\rho|} + \tfrac{1}{2} - k^2\right)\theta_i(\bar{\sigma}+\tfrac{1}{2}\bar{\rho},\bar{\sigma}-\tfrac{1}{2}\bar{\rho})$$

$$H_{ij} = \int d\bar{r}d\bar{r}_p\ \theta_i(\bar{r},\bar{r}_p) H \theta_j(\bar{r},\bar{r}_p)$$

and the evaluation of the functions $\mathcal{G}_0$ etc. in $\mathcal{K}_{12}^{cs}$ as given by (A.3), the integrations have to be carried out numerically.

Having obtained the matrix elements H_{ij} and the overlaps N_{ij}, the eigenvalue problem of (2.22), when written in matrix form, becomes

$$\tilde{H}\bar{a} = \varepsilon\tilde{N}\bar{a} \; . \tag{4.2}$$

Noting $\tilde{N}$ being symmetric and positive definite, one can find a lower triangular matrix $\tilde{L}$ such that $\tilde{L}\tilde{L}^T = \tilde{N}$ (58). Equation (4.2) now becomes

$$\tilde{H}\bar{a} = \varepsilon\tilde{L}\tilde{L}^T\bar{a} \tag{4.3}$$

Multiplying (4.3) from the left by $\tilde{L}^{-1}$ and inserting

$$\tilde{I} = \tilde{L}^{T^{-1}}\tilde{L}^T = \tilde{L}^{-1^T}\tilde{L}^T$$

between $\tilde{H}$ and $\bar{a}$, we get

$$(\tilde{L}^{-1}\tilde{H}\tilde{L}^{-1^T})(\tilde{L}^T\bar{a}) = \varepsilon\tilde{L}^T\bar{a}$$

which can readily be identified as the more familiar eigenvalue equation

$$\tilde{A}\bar{x} = \varepsilon\bar{x} \tag{4.4}$$

with $\tilde{A} = \tilde{L}^{-1}\tilde{H}\tilde{L}^{-1^T}$ and $\bar{x} = \tilde{L}^T\bar{a}$. With $\tilde{A}$ being symmetric (4.4) can be solved by the standard procedure of Jacobi's method (59). The eigenvalues ε from (4.4) are the same as those from (4.2), while the eigenvectors $\bar{a}$ of the original problem (4.2) can be easily obtained from the relation $\bar{a} = (\tilde{L}^{-1})^T\bar{x}$.

With all the eigenvectors $\bar{a}^{\lambda} = \left(a_i^{\lambda}\right)$, each corresponding to an eigenvalue ε^{λ}, known, $\mathcal{V}^{\lambda}(r_p)$ and $\mathcal{W}^{\lambda}(\sigma)$ of (2.28) can be formed from $\mathcal{V}_i(r_p)$ and $\mathcal{W}_i(\sigma)$ already evaluated, by

$$\begin{aligned} \mathcal{V}^{\lambda}(r_p) &= \sum_i a_i^{\lambda} \mathcal{V}_i(r_p) \\ \mathcal{W}^{\lambda}(\sigma) &= \sum_i a_i^{\lambda} \mathcal{W}_i(\sigma) \cdot \end{aligned} \tag{4.5}$$

Now the kernels in (2.28), namely

$$\begin{aligned} \mathcal{K}_{11}(r_p, r_p') &= \sum_{\lambda} \frac{\mathcal{V}^{\lambda}(r_p)\, \mathcal{V}^{\lambda}(r_p')}{E - \varepsilon^{\lambda}} \\ \mathcal{K}_{12}(r_p, \sigma) &= \sum_{\lambda} \frac{\mathcal{V}^{\lambda}(r_p)\, \mathcal{W}^{\lambda}(\sigma)}{E - \varepsilon^{\lambda}} + \mathcal{K}_{12}^{cs}(r_p, \sigma) \\ &= \mathcal{K}_{21}(r_p, \sigma) \\ \mathcal{K}_{22}(\sigma, \sigma') &= \sum_{\lambda} \frac{\mathcal{W}^{\lambda}(\sigma)\, \mathcal{W}^{\lambda}(\sigma')}{E - \varepsilon^{\lambda}} \quad , \end{aligned} \tag{4.6}$$

are all known. We then proceed to solve the system of integro-differential equations

$$\begin{aligned} \left(\frac{d^2}{dr_p^2} + k^2\right) f(r_p) &= U(r_p) f(r_p) + \int_0^{\infty} dr_p'\, \mathcal{K}_{11}(r_p, r_p') f(r_p') \\ &\quad + \int_0^{\infty} d\sigma'\, \mathcal{K}_{12}(r_p, \sigma') g(\sigma') \\ \left(\frac{d^2}{d\sigma^2} + \kappa^2\right) g(\sigma) &= 2\int_0^{\infty} dr_p'\, \mathcal{K}_{21}(r_p', \sigma) f(r_p') \\ &\quad + 2\int_0^{\infty} d\sigma'\, \mathcal{K}_{22}(\sigma, \sigma') g(\sigma') \end{aligned} \tag{4.7}$$

with the boundary conditions

$$
\begin{aligned}
& f_\nu(0) = g_\nu(0) = 0 \quad , \qquad \nu = 1,2 \\
& f_1(r_p) \sim \sin(kr_p) + R_{11}\cos(kr_p) \\
& g_1(\sigma) \sim \sqrt{\left(\frac{2k}{\kappa}\right)}\, R_{21}\cos(\kappa\sigma) \\
& f_2(r_p) \sim \sqrt{\left(\frac{\kappa}{2k}\right)}\, R_{12}\cos(kr_p) \\
& g_2(\sigma) \sim \sin(\kappa\sigma) + R_{22}\cos(\kappa\sigma) \quad , \qquad \text{for } k^2 \geq \tfrac{1}{2}
\end{aligned}
\tag{4.8}
$$

and

$$
\begin{aligned}
& f(r_p) \sim \sin(kr_p) + \tan\eta_o \cos(kr_p) \\
& g(\sigma) \sim \alpha \exp(-|\kappa|\sigma) \quad , \quad \text{for } k^2 < \tfrac{1}{2} \ .
\end{aligned}
\tag{4.9}
$$

Once f and g are solved, the coefficients c_i in the trial wave function (2.13) are obtained from (2.23) and (2.24), namely

$$
c_i = \sum_{\lambda=1}^{n} a_i^\lambda b^\lambda \tag{4.10}
$$

and

$$
b^\lambda = \frac{\sqrt{4\pi}}{E-\varepsilon^\lambda}\left\{\int_0^\infty dr_p\, \mathcal{U}^\lambda(r_p) f(r_p) + \int_0^\infty d\sigma\, \mathcal{W}^\lambda(\sigma) g(\sigma)\right\} \ . \tag{4.11}
$$

The Coupled Integral Equations

The system (4.7) with (4.8) can be transformed into integral equations by using the appropriate Green's functions as

$$f_\nu(r_p) = \delta_{1\nu}\sin(kr_p) + \int_0^\infty dr_p'\, G(r_p,r_p')\,\{\, U(r_p')f(r_p') + \int_0^\infty dr_p''\, \mathcal{K}_{11}(r_p',r_p'')f(r_p'') + \int_0^\infty d\sigma'\, \mathcal{K}_{12}(r_p',\sigma')g(\sigma')\,\}$$

$$g_\nu(\sigma) = \delta_{2\nu}\sin(\kappa\sigma) + \int_0^\infty d\sigma'\, O(\sigma,\sigma')\,\{ \; 2\int_0^\infty dr_p'\, \mathcal{K}_{21}(r_p',\sigma')f(r_p') + 2\int_0^\infty d\sigma''\, \mathcal{K}_{22}(\sigma',\sigma'')g(\sigma'')\,\} \tag{4.12}$$

where

$$G(r_p,r_p') = \begin{cases} -\frac{1}{k}\sin(kr_p')\cos(kr_p) & (r_p' \le r_p) \\ -\frac{1}{k}\sin(kr_p)\cos(kr_p') & (r_p' \ge r_p) \end{cases} \tag{4.13}$$

and

$$O(\sigma,\sigma') = \begin{cases} -\frac{1}{\kappa}\sin(\kappa\sigma')\cos(\kappa\sigma) & (\sigma' \le \sigma) \\ -\frac{1}{\kappa}\sin(\kappa\sigma)\cos(\kappa\sigma') & (\sigma' \ge \sigma)\ . \end{cases} \tag{4.14}$$

For energies in the elastic region $k^2 < \tfrac{1}{2}$, $\kappa^2 = 2k^2 - 1$ is negative. Equation (4.7) with (4.9) is now transformed into

$$f(r_p) = \sin(kr_p) + \int_0^\infty dr_p'\, G(r_p,r_p')\{Uf+\dots\}$$

$$g(\sigma) = \int_0^\infty d\sigma' O(\sigma,\sigma')\,\{.. + ..\} \tag{4.15}$$

with $G(r_p,r_p')$ remaining the same as in (4.13), while $O(\sigma,\sigma')$ is now given by

$$O(\sigma,\sigma') = \begin{cases} -\frac{1}{|\kappa|}\sinh(|\kappa|\sigma')\exp(-|\kappa|\sigma) & (\sigma' \le \sigma) \\ -\frac{1}{|\kappa|}\sinh(|\kappa|\sigma)\exp(-|\kappa|\sigma') & (\sigma' \ge \sigma) \end{cases} \tag{4.16}$$

At the zero energy limit, as $k^2 \to 0$, (4.7) becomes asymptotically

$$\frac{d^2}{dr_p^2} f(r_p) = 0 ,$$

and

$$f(r_p) \sim r_p - a . \tag{4.17}$$

a is the scattering length, and the cross-section is given by

$$\sigma_{11} = 4a^2 . \tag{4.18}$$

The scattering length a can be determined by the method given, for example, by Fraser[60]. Defining

$$u(r_p) = \left(\frac{f(r_p)}{k}\right)_{k^2 \to 0} \quad \text{and} \quad v(\sigma) = \left(\frac{g(\sigma)}{k}\right)_{k^2 \to 0} , \tag{4.19}$$

the first of (4.15) can be written as

$$u(r_p) = r_p + \int_0^\infty dr_p' G(r_p, r_p') \{Uu + \int \mathcal{K}_{11} u + \int \mathcal{K}_{12} v \} \tag{4.20}$$

with

$$G(r_p, r_p') = \begin{cases} -r_p' & (r_p' \leq r_p) \\ -1 & (r_p' \geq r_p) \end{cases} \tag{4.21}$$

The second equation of (4.15) remains unchanged except by putting u and v in place of f and g. The scattering length is then determined from the asymptotic region of u.

Iterative Method

We can attempt to solve Equations (4.12), (4.15) and (4.20) iteratively. To be specific, let us consider (4.15).

Essentially the iterative method of McEachran and Fraser[61] consists of first evaluating the right hand side of (4.15) with an initial guess of $\begin{pmatrix} f \\ g \end{pmatrix}^{(0)} = \begin{pmatrix} \sin(kr_p) \\ 0 \end{pmatrix}$ giving a $\begin{pmatrix} f \\ g \end{pmatrix}^{(1)}$ on the left hand side. From the asymptotic region of $\begin{pmatrix} f \\ g \end{pmatrix}^{(1)}$, one gets $\tan \eta_o^{(1)}$. $\begin{pmatrix} f \\ g \end{pmatrix}^{(1)}$ is again put into the right hand side to give a $\begin{pmatrix} f \\ g \end{pmatrix}^{(2)}$ and $\tan \eta_o^{(2)}$ and so on. This process is repeated until $| 1 - \tan \eta_o^{(n)} / \tan \eta_o^{(n-1)} |$ is less than a prescribed epsilon, where n is the iteration number. Convergence is said to have been obtained, and $\begin{pmatrix} f \\ g \end{pmatrix}^{(n)}$ is taken as the solution to (4.15).

This method has been applied to solve (4.12) and (4.15). Unfortunately, even with other variants of the method[62] or with the variational iterative method of McEachran et al[63], no convergence has been obtained except for (4.15) in the coupled static approximation.

Conversion to A System of Linear Equations

With the iterative method failing to work, we now proceed to seek another way to solve the coupled integral equation (4.15) which we take again as an illustrative example. From now on, for simplicity, the subscript p in r_p will be dropped. All the integrations involved are approximated by some numerical rules, paying particular attention to use the same rule, using n_f points, for all the r-integrations in which the integrands contain the unknown

function f(r). Similarly, we do the same to the σ-integration using n_g points for the integrals involving the function g(σ). Thus (4.15) is now approximated by

$$f_i = s_i + \sum_j G_{ij}\alpha_j U_j f_j + \sum_{k,j} G_{ik}\gamma_k \mathcal{K}^{11}_{kj}\alpha_j f_j + \sum_{\ell,j'} G_{i\ell}\delta_\ell \mathcal{K}^{12}_{\ell j'}\beta_{j'}g_{j'},$$

$$g_{i'} = \sum_{j',j} O_{i'j'}\varepsilon_{j'}\mathcal{K}^{21}_{jj'}\alpha_j f_j + \sum_{k',j} O_{i'k'}\lambda_{k'}\mathcal{K}^{22}_{k'j'}\beta_{j'}g_{j'}, \tag{4.22}$$

where α_j are the numerical integration weights in the r-integration involving f, and $f_j = f(r_j)$ are the functional values of f at the corresponding abscisae r_j. The other symbols are similarly defined. Note the unprimed and primed indices are referring to the r- and σ-integration respectively, and the weights α_j and $\beta_{j'}$ go with f_j and $g_{j'}$.

Equations (4.22) may be rewritten in matrix notation as

$$\bar{y} = \bar{s} + \tilde{M}\bar{y} \qquad \text{or} \qquad (\tilde{M} - \tilde{I})\bar{y} = -\bar{s} \tag{4.23}$$

where $\bar{y} = \begin{pmatrix} \vdots \\ f_i \\ \vdots \\ g_{i'} \\ \vdots \end{pmatrix}$ and $\bar{s} = \begin{pmatrix} \vdots \\ s_i \\ \vdots \\ 0 \\ \vdots \end{pmatrix}$

are column vectors of dimension $n = n_f + n_g$, and

$$\tilde{M} = \begin{pmatrix} M_{ij} & \vdots & M_{ij'} \\ \cdots & \vdots & \cdots \\ M_{ji'} & \vdots & M_{j'j'} \\ & \vdots & \end{pmatrix}$$

is an n x n square matrix written in terms of the submatrices

$\tilde{M}_{ij}$ etc. whose coefficients can easily be identified with some of the expressions in (4.23), and $\tilde{I}$ is the n x n unit matrix.

The system (4.23) of linear algebraic equations can readily be solved by a standard Gaussian elimination procedure, giving the solution $\bar{y} = \begin{pmatrix} f_i \\ g_i \end{pmatrix}$ from the asymptotic form of which tan η_0 can be determined. Explicitly,

$$\tan \eta_0 = (f_j - s_j)/c_j \tag{4.24}$$

where j denotes some point in the asymptotic region, and $c_j = \cos(kr_j)$. Since f satisfies

$$f(r) = \sin(kr) + \int_0^\infty dr' G(r,r')\{Uf + \int \mathcal{K}_{11} f + \int \mathcal{K}_{12} g\}$$

and

$$G(r,r') = -\frac{1}{k} \cos(kr)\sin(kr') \quad , \quad \text{for large } r,$$

one can see that the value of tan η_0 given by (4.24) would be the same as that obtained from the integral expression

$$\tan \eta_0 = -\frac{1}{k} \int_0^\infty dr' \sin(kr')\{Uf + \int \mathcal{K}_{11} f + \int \mathcal{K}_{12} g\}$$

Also one can obtain the annihilation parameter Z_{eff} as given by (3.10), as all the integrals can be evaluated analytically or numerically using the values of f_j and g_j, .

This method is used in solving (4.12),(4.15) and (4.20) corresponding to different energy regions. For the inelastic case (4.12), we have two systems of equations, one for each solution,

$$(\tilde{M} - \tilde{I}) \bar{y}_\nu = - \bar{s}_\nu \qquad \nu = 1,2 \qquad (4.25)$$

with

$$\bar{s}_1 = \begin{pmatrix} \vdots \\ \sin(kr_i) \\ \vdots \\ 0 \\ \vdots \end{pmatrix} \quad \text{and} \quad \bar{s}_2 = \begin{pmatrix} \vdots \\ 0 \\ \vdots \\ \sin(\kappa\sigma_{i'}) \\ \vdots \end{pmatrix}$$

The solutions $\bar{y}$ from the two systems can be obtained at the same time during the elimination procedure, since we have the same coefficient matrix $(\tilde{M}-\tilde{I})$ for both systems. The R-matrix elements are again determined from the asymptotic regions of the solutions $\bar{y}_\nu = \begin{pmatrix} f \\ g \end{pmatrix}_\nu$ as

$$R_{11} = (f_1(r_j) - \sin(kr_j))/\cos(kr_j)$$

$$R_{12} = \sqrt{(\frac{2k}{\kappa})}\ f_2(r_j)/\cos(kr_j) \qquad \text{, for some large } r_j, \qquad (4.26)$$

and

$$R_{21} = \sqrt{(\frac{\kappa}{2k})}\ g_1(\sigma_{j'})/\cos(\kappa\sigma_{j'})$$

$$R_{22} = (g_2(\sigma_{j'}) - \sin(\kappa\sigma_{j'}))/\cos(\kappa\sigma_{j'}) \quad ,$$

for some large $\sigma_{j'}$.

Integration Formulas Used

All numerical integrations are done using Gaussian quadrature for integrals with finite limits, and the Gauss-Laguerre formula, when the upper limit is infinite. An n-point Gaussian quadrature would give an exact evaluation of the integral if the integrand were a polynomial

of degree (2n-1) or lower[59]. Also for an n-point Gauss Laguerre formula the integral $\int_0^\infty dx P_{2n-1}(x)\exp(-x)$, where $P_{2n-1}(x)$ is a polynomial of (2n-1) degree, is evaluated exactly. Here we can use the latter formula because in all our integrals the integrands decay like $\exp(-\alpha x)$ at large x. The factor α can be removed by a simple scaling; for α not too much different from unity, it does not affect the accuracy too much so long as a high enough n is used. The range of integration is from 0 to ∞ in all cases. It is broken into smaller regions, starting or ending at points where the integrand has a discontinuity in slope, or at some arbitrarily chosen point to subdivide the range into smaller regions so as to achieve better accuracy.

Numerical Details

For the r-integration involving f, a 20-point Gauss-Legendre formula is used to cover the range from 0 to $4a_o$, and a 20-point Gauss-Laguerre formula, from $4a_o$ to ∞ . We do the same for the σ-integration involving g for the same first region, but use 15 Gauss-Laguerre points for the latter range. This is because, for the values of λ_i and μ_i used in our choice of the θ_i in (2.13), some of the potentials $\mathcal{U}_i(r)$ are of quite long range, while the $\mathcal{W}_i(\sigma)$ are much shorter. So for our system of linear algebraic equations (4.23), we have 40 points of f_i and 35 points of g_i, to solve, making the total dimension of the system 75x75.

The potentials $V_i(r)$ and $W_i(\sigma)$ making up the kernels are evaluated at the Gaussian points and each stored in the computer in two parts, the energy-independent and energy-dependent part, as, for example, $V_i = V_i^{ind} + k^2 V_i^{dep}$, so that V_i can be formed readily for any energy we want; and from them we can get $V^{\lambda}(r)$ and $W^{\lambda}(\sigma)$ using (4.5).

The computer program subroutines for solving the transformed eigen value problem (4.4) by Jacobi's method and the system of linear equations (4.23) by the Gauss-Jordan method are obtained from the Computing Centre of the university. All programs were written in FORTRAN, created and debugged using the DEC-PDP10 cited at this university. The final computations were done on the CDC6600 at Multiple Access General Computer Corporation, Don Mills, Ontario. The shift from the PDP10 to the CDC6600 was made after the discovery that the 36-bit word length of the PDP10 does not provide enough accuracy for some of the calculations. The latter machine has a 60-bit word length, giving 14 significant figures at single precision.

Check on Accuracy

It can be shown that the approximate R-matrix from (4.7) is, like the exact one, symmetric. Since (4.7) is transformed into the integral equation (4.15) which is numerically approximated by (4.25), the solution of which with $\bar{s}_1 = \begin{pmatrix} \sin(kr) \\ 0 \end{pmatrix}$ gives R_{11} and R_{21} and with $\bar{s}_2 = \begin{pmatrix} 0 \\ \sin(\kappa\sigma) \end{pmatrix}$ gives R_{12} and R_{22},

the symmetry of R is not obvious at all. In fact a comparison of R_{12} and R_{21} obtained from (4.25) reflects the accuracy of the numerical work.

Another independent check on the numerical accuracy and on the programming is provided by the identity described below.

Let s(r) and t(σ) be the solution of

$$\left(\frac{d^2}{dr^2} + k^2\right) s(r) = U(r)s(r) + \int_0^\infty d\sigma' \mathcal{K}_{12}^{cs}(r,\sigma') t(\sigma')$$

$$\left(\frac{d^2}{d\sigma^2} + \kappa^2\right) t(\sigma) = 2\int_0^\infty dr' \mathcal{K}_{12}^{cs}(r',\sigma) s(r')$$

coming from the coupled static approximation, with boundary conditions being the same as those given in (4.8) for f and g, but with R replaced by R^{cs}. One can easily establish the identity

$$R_{\nu\nu'} - R^{cs}_{\nu\nu'} = -\frac{1}{\sqrt{k_\nu k_{\nu'}}} \sum_\lambda \frac{1}{(E - \varepsilon^\lambda)} \Big\{ \Big\{ \int_0^\infty dr\, \mathcal{V}^\lambda(r) f_\nu(r) + \int_0^\infty d\sigma\, \mathcal{W}^\lambda(\sigma) g_\nu(\sigma) \Big\} \Big\{ \int_0^\infty dr\, \mathcal{V}^\lambda(r) s_{\nu'}(r) + \int_0^\infty d\sigma\, \mathcal{W}^\lambda(\sigma) t_{\nu'}(\sigma) \Big\} \Big\} . \tag{4.27}$$

It gives the increment of the R-matrix elements from the coupled static approximation value R^{cs} in terms of the kernels introduced by the correlation terms, as well as the solutions $\begin{pmatrix} s(r) \\ t(\sigma) \end{pmatrix}_{\nu'}$ and $\begin{pmatrix} f(r) \\ g(\sigma) \end{pmatrix}_{\nu}$. We have a similar relation for the tan η_0 in the elastic case (see e.g.

Ref.(1)), and the scattering length a in the zero energy limit.

CHAPTER V

RESULTS

Theoretically speaking, any choice of θ_i in the trial wave function (2.13) will give a bound to the R-matrix for energies below ε_o so long as it does not contribute to the total wave function in the asymptotic region. Also, by increasing n, the number of terms used in the expansion, one can get as close to the exact R-matrix as desired. Yet in practice, one has to limit oneself to some finite n: here we stop at n=26. Furthermore, for a given n, one can vary the nonlinear parameters λ and μ in the expression for θ_i given in (4.1) to get better (higher) phase shifts or $R_{\nu\nu}$ for each energy. Such a procedure would be very time consuming.

A preliminary survey using only ten terms all with the same λ and μ was carried out for several energies to find out the range of their values for best results. It turns out that their choice is not too critical, and that it depends also on energy. Accordingly, the values of λ and μ are chosen appropriately using the survey as a guide. The value of λ=0.5 in some θ are chosen to simulate the 2s and 2p states of hydrogen which might be important to produce a resonance. Once chosen, the same 26 terms are used for all energies. The factor $P_\ell(\hat{r}.\hat{r}_p)$ is put in to give some additional angular dependence of θ_i on the angle between the

positron and electron coordinates. The parameters specifying each θ_i for i=1,26 are shown in Table I.

Elastic Region

The phase shift in the elastic region serves the purpose of giving a check on the usefulness of the correlation functions rather than presenting a set of new results, as accurate and reliable lower bound estimates of the phase shift have already been obtained by Bhatia et al[1]. It would be too much to list all the work in this energy region, for reason of clarity, only a few are included. The results of the coupled static approximation (in this energy region, it is also called the 'static+virtual positronium formation'), and those with 26 correlation terms are listed in Table II as (d) and (b) respectively, together with (a) the accurate results of Ref. (1), (c) the static approximation, (e) the 6-hydrogenic-state eigen function expansion of McEachran and Fraser[21] and (f) the pseudo-state expansion (H(1s)-H($\overline{2p}$)-Ps(1s)-Ps($\overline{2p}$)) of Wakid and LaBahn[32] (their appr.(e)).

To evaluate the usefulness of each calculation, Drachman[23] has introduced a figure of merit, or quality factor Q, defined as $Q(k) = (\eta_0(k) - \eta_0^s(k))/(\eta_0^{Bh}(k) - \eta_0^s(k))$, where η_0 is the calculated phase shift, η_0^s and η_0^{Bh} are the phase shifts from the static approximation, and those of Bhatia et al[1]. The usefulness of an approximation is reflected by how close Q is to unity. During the initial survey of the choice of the parameters λ and μ, it was

TABLE I

Parameters of the Functions θ_i

i	α_i	β_i	γ_i	λ_i	μ_i	ℓ_i
1	0	0	0	.8	.5	0
2	0	0	1	.9	.6	0
3	0	1	0	.9	.4	0
4	1	0	0	.9	.4	0
5	1	1	0	.8	.5	0
6	1	0	1	.8	.5	0
7	0	1	1	.8	.5	0
8	1	1	1	.9	.6	0
9	1	1	0	.9	.6	1
10	1	1	1	.9	.6	1
11	0	0	0	.6	.6	0
12	1	0	1	1.1	.8	0
13	0	1	1	1.1	.8	0
14	1	1	1	1.1	.8	0
15	0	0	0	.5	.5	0
16	0	0	1	.5	.5	0
17	0	1	0	.5	.5	0
18	1	0	0	.5	.5	0
19	1	1	0	.5	.5	1
20	1	1	1	.5	.5	1
21	0	0	2	.8	.5	0
22	0	2	0	.8	.5	0
23	2	0	0	.8	.5	0
24	0	0	0	.5	.4	0
25	1	0	0	.5	.4	0
26	1	1	0	.5	.4	0

$$\theta_i = r^{\alpha_i} r_p^{\beta_i} \rho^{\gamma_i} \exp(-\lambda_i r - \mu_i r_p)\ P_{\ell_i}(\hat{r}.\hat{r}_p)$$

TABLE II

S-Wave Phase Shifts

k	(a)	(b)	(c)	(d)	(e)	(f)
0	-2.10	-1.70	.582	.172		-.94
.1	.1483	.140	-.058	-.019	.007	
.2	.1877	.182	-.118	-.047	-.025	.055
.3	.1677		-.168		-.075	
.4	.1201	.114	-.218	-.137	-.130	
.5	.0624	.056	-.264	-.186	-.183	
.6	.0039	-.005	-.304	-.242	-.232	-.157
.7	-.0512	-.060		-.290		-.209

The row at k=0 shows scattering length

(a) Bhatia et al[1]

(b) present calculation

(c) static approximation

(d) coupled static approximation

(e) (1s-2s-2p-3s-3p-3d), McEachran and Fraser[21]

(f) (H(1s)-H($\overline{2p}$)-Ps(1s)-Ps($\overline{2p}$)),
Wakid and LaBahn[32] (their approx.(e))

found that with only a few terms, the phase shifts climbed up from the poor value of the coupled static approximation to give a quality factor of over 90% easily. With 26 terms, a Q value of 98% is obtained for $k \geq 0.2$, and 96% at $k = 0.1$. The Q value for the 6-state calculation of Ref.(21) and the pseudo-state calculation of Ref.(32) are about 30% and 60% respectively. This demonstrates clearly that short range correlation terms can represent the closed channel part of Ψ much better than the higher target states or the pseudo-state expansion which takes specifically the virtual excitation or polarization of the target atom into consideration.

A direct calculation of u and v defined in (4.19) at $k^2 = 0$, gives $a = -1.70$ as compared to the value of -2.10 obtained by Bhatia et al[1]. The coupled static approximation gives $a = 0.170$. The correlation functions are not as 'useful' at zero energy as they are at non-zero energies. This may be due to the fact that at very low energies, the polarization of the target becomes important, and the choice of θ_i does not allow for this fully.

A plot of phase shifts against momentum k is shown in Fig. I.

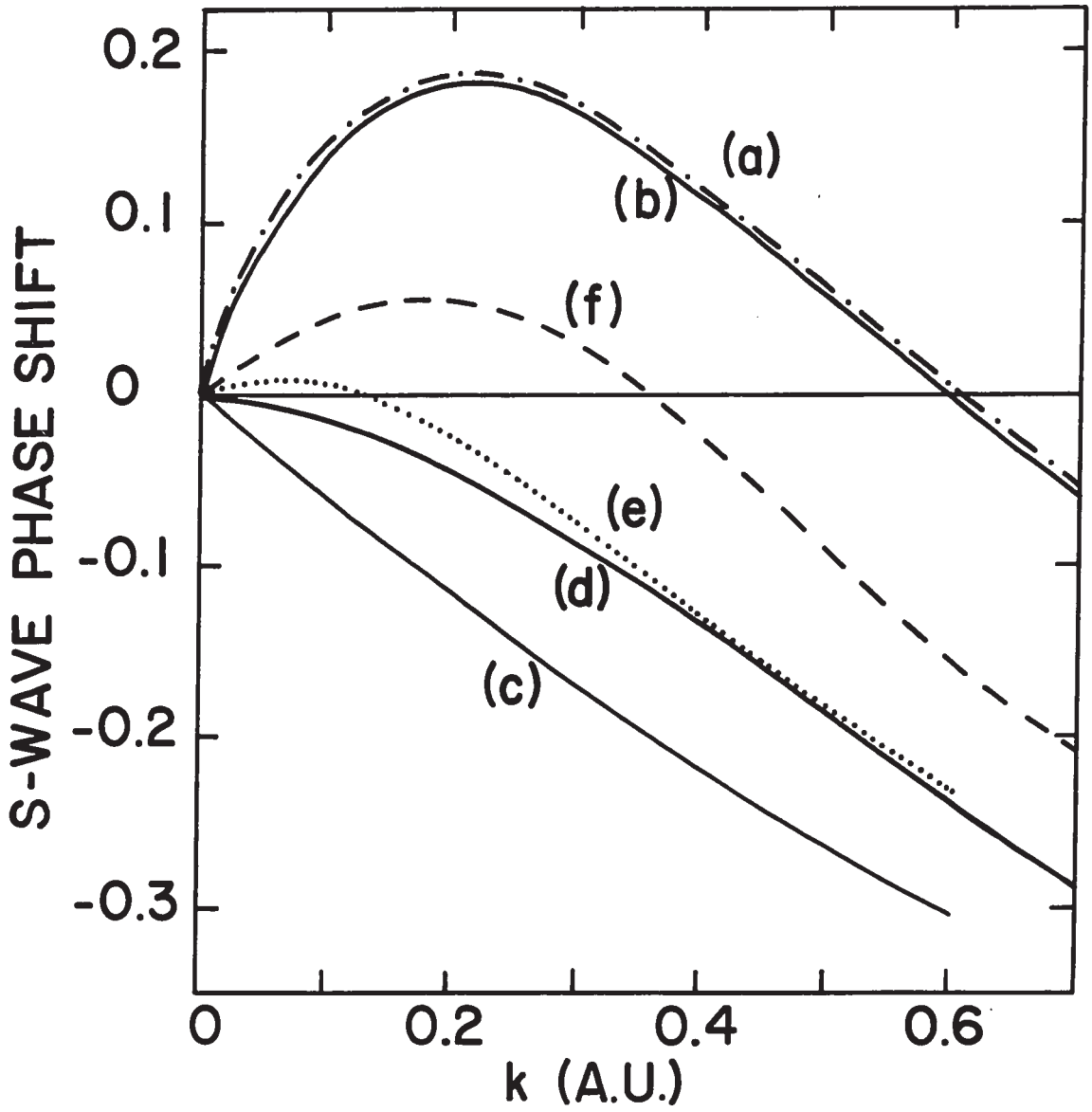

Fig.I S-Wave Phase Shifts. (a),Bhatia et al[1]; (b),present calculation; (c), static; (d), coupled static; (e),(1s-2s-2p-3s-3p-3d), McEachran and Fraser[21]; (f), ($H(1s)-H(\overline{2p})-Ps(1s)-Ps(\overline{2p})$), Wakid and LaBahn[32] (their approx.(e)).

Inelastic Region

The R-matrix from the coupled static approximation obtained in this work agrees very well with that obtained by Cody et al[14], Dirks and Hahn[64] and Wakid and LaBahn[32]. This agreement gives a check on the method employed and the accuracy of the numerical work. This approximation totally neglects the closed channel part of Ψ, but still provides a lower bound to the R-matrix. The only other reported calculation that gives a bound is that by Dirks and Hahn[41] who apply the formalism of the generalized variational bounds[40] to this problem. With 26 terms, the present calculation gives higher diagonal R-matrix elements and higher eigen phases than those obtained by Ref.(41). Although the bound principle is only true for energies below the lowest eigenvalue ε_o, of QHQ, which has not yet been found, yet based on the finding of Hahn and Dirks[45], it is likely to be very near to the n=2 excitation threshold of hydrogen if one exists below at all. Granting this to be true, the present calculated values of $R_{\nu\nu}$ and eigen phases are lower bounds to the exact ones up to energies very close to the threshold.

Table III shows the R-matrix obtained by the present calculations (a) and (c), and by others including (b) the bound calculation of Ref.(41), and (d) the pseudo-states (H(1s)-H($\overline{2p}$)-Ps(1s)-Ps($\overline{2p}$) calculation of Wakid and LaBahn[32]. The formulation in the latter work does not satisfy a bound principle.

TABLE III

R-matrix Elements and Eigen Phases

k		R_{11}	$R_{12}=R_{21}$	R_{22}	δ_1	δ_2
.71	(a)	-.0651	-.0136	-.0792	-.057	-.087
	(c)	-.304	-.0005	-.268	-.262	-.295
.75	(a)	-.0862	-.025	-.7227	-.085	-.626
	(b)	-.133	-.0027	-.805	-.132	-.678
	(c)	-.323	-.0052	-1.486	-.312	-.978
	(d)	-.315	-.048	-.472	-.293	-.452
.80	(a)	-.111	-.047	-1.854	-.110	-1.08
	(b)	-.159	-.0087	-2.448	-.158	-1.18
	(c)	-.347	-.035	-5.490	-.334	-1.39
	(d)	-.339	-.065	-.586	-.312	-.542
.85	(a)	-.137	-.132	-5.354	-.133	-1.39
	(b)	-.185	-.105	-19.71	-.182	-1.52
	(c)	-.367	.104	10.20	-.353	-1.67
	(d)	-.366	-.092	-.344	-.257	-.420
.866	(a)	-.146	-.243	-9.662	-.140	-1.47

(a) present calculation
(b) Dirks and Hahn[41]
(c) coupled static
(d) (H(1s)-H($\overline{2p}$)-Ps(1s)-Ps($\overline{2p}$)), Wakid and LaBahn[32] (their approx.(e))

As n is increased in steps of one from 23 to 26, R_{11} elements change by less than .2%. For R_{12}, R_{21} and R_{22}, they change by less than a few percent. These changes are surely very small compared to the jump we have from the coupled static values to the final results. This shows some sort of convergence has been reached.

The T-matrix of this and other above mentioned calculations obtained from the R-matrices using (2.7) are presented in Table IV which also includes the results of Doolen et al[65] who calculate the T_{11} element of the T-matrix in the complex energy plane and extrapolate back to real energies. In the elastic region they have obtained phase shifts very close to those of Bhatia et al[1]. As can be seen from Table IV, their T_{11} elements are in good agreement with those from the present calculation. Since for the calculation of T_{11} all four elements of the R-matrix are involved, this agreement adds support to the results in the inelastic region.

TABLE IV

Real and Imaginary Parts of T-Matrix Elements

k		T_{11}		$T_{12}=T_{21}$		T_{22}	
		Re	Im	Re	Im	Re	Im
.75	(a)	.016	.170	.263	.031	.686	.949
	(b)	.035	.261	.003	.003	.786	.977
	(c)	.189	.585	.005	.002	1.37	.926
	(d)	.182	.570	.056	.061	.366	.769
.80	(a)	.025	.218	.042	.017	1.55	.835
	(b)	.049	.310	.006	.002	1.71	.700
	(c)	.215	.619	.012	-.002	1.94	.353
	(d)	.209	.602	.080	.070	.512	.867
	(e)	.028	.196				
.85	(a)	.036	.262	.048	.003	1.93	.361
	(b)	.066	.357	.010	-.001	1.99	.101
	(c)	.239	.649	.017	-.008	1.98	-.194
	(d)	.244	.634	.102	.127	.219	.603
	(e)	.036	.245				

(a) present calculation
(b) from R-matrix of Dirks and Hahn[41]
(c) coupled static
(d) from R-matrix of Wakid and LaBahn[32], (their approx.(e))
(e) Doolen et al[65], (their T by -2i)

Cross Sections

Cross sections in the inelastic region are calculated from the R-matrix using (2.9). They are shown in Table V. For comparison, values from the calculations of Dirks and Hahn[41] and Wakid and LaBahn[32] at k = .75, .80, and .85 are also included. Since R_{11} are lower bounds and are negative, the elastic cross sections σ_{11} are probably upper bounds, as remarked also by Dirks and Hahn[41].

Fig. II displays the elastic cross sections in units of πa_o^2. Curve (a) represents the results from the phase shifts of Bhatia et al[1]. Curve (b) is the present calculation with 26 correlation terms, and (c), the coupled static approximation. Results of Dirks and Hahn[41] and a pseudo-state expansion (H(1s)-H($\overline{2p}$)-Ps(1s)-Ps($\overline{2p}$)) calculation of Wakid and LaBahn[32] (their approx. (e)) are shown in curve (e) and (d). Other reported works in this energy region are those of Bransden and Jundi[36] and Fels and Mittleman[38]. They have investigated in different approximations and models the effects of the polarization of the hydrogen and positronium atoms. Their results change considerably with the approximations and models used. Curve (f) shows the result of approximation B(1) of Ref.(36), and (g) that of model (V) of Ref.(38). Curve (b) of the present calculation runs very closely to (a) of Bhatia et al[1] in the elastic region, and joins continuously at threshold to the inelastic region.

TABLE V

Cross Sections in Units of πa_o^2

k	k^2		σ_{11}	σ_{12}	σ_{21}	σ_{22}
.71	.5041		.335(-1)	.15(-2)	.89(-2)	3.04
.72	.5184		.381(-1)	.24(-2)	.33(-1)	6.12
.73	.5329		.427(-1)	.27(-2)	.22(-1)	8.48
.74	.5476		.474(-1)	.28(-2)	.16(-1)	10.00
.75	.5625		.521(-1)	.29(-2)	.13(-1)	10.97
		(a)	.124	.3 (-4)	.14(-3)	12.58
		(b)	.636	.12(-1)	.55(-1)	5.80
.80	.64		.752(-1)	.31(-2)	.72(-2)	11.05
		(a)	.154	.66(-4)	.15(-3)	12.24
		(b)	.634	.18(-1)	.40(-1)	3.62
.83	.6889		.884(-1)	.31(-2)	.57(-2)	9.67
.85	.7225		.967(-1)	.32(-2)	.52(-2)	8.68
		(a)	.182	.15(-3)	.25(-3)	8.97
		(b)	.638	.37(-1)	.59(-1)	.93
.86	.7396		.101	.32(-2)	.50(-2)	8.19
.866	.74996		.103	.33(-2)	.49(-2)	7.91

The numbers in parenthesis indicate the power of 10 to be multiplied. (a) and (b) are results of Dirks and Hahn[41] and Wakid and LaBahn[32].

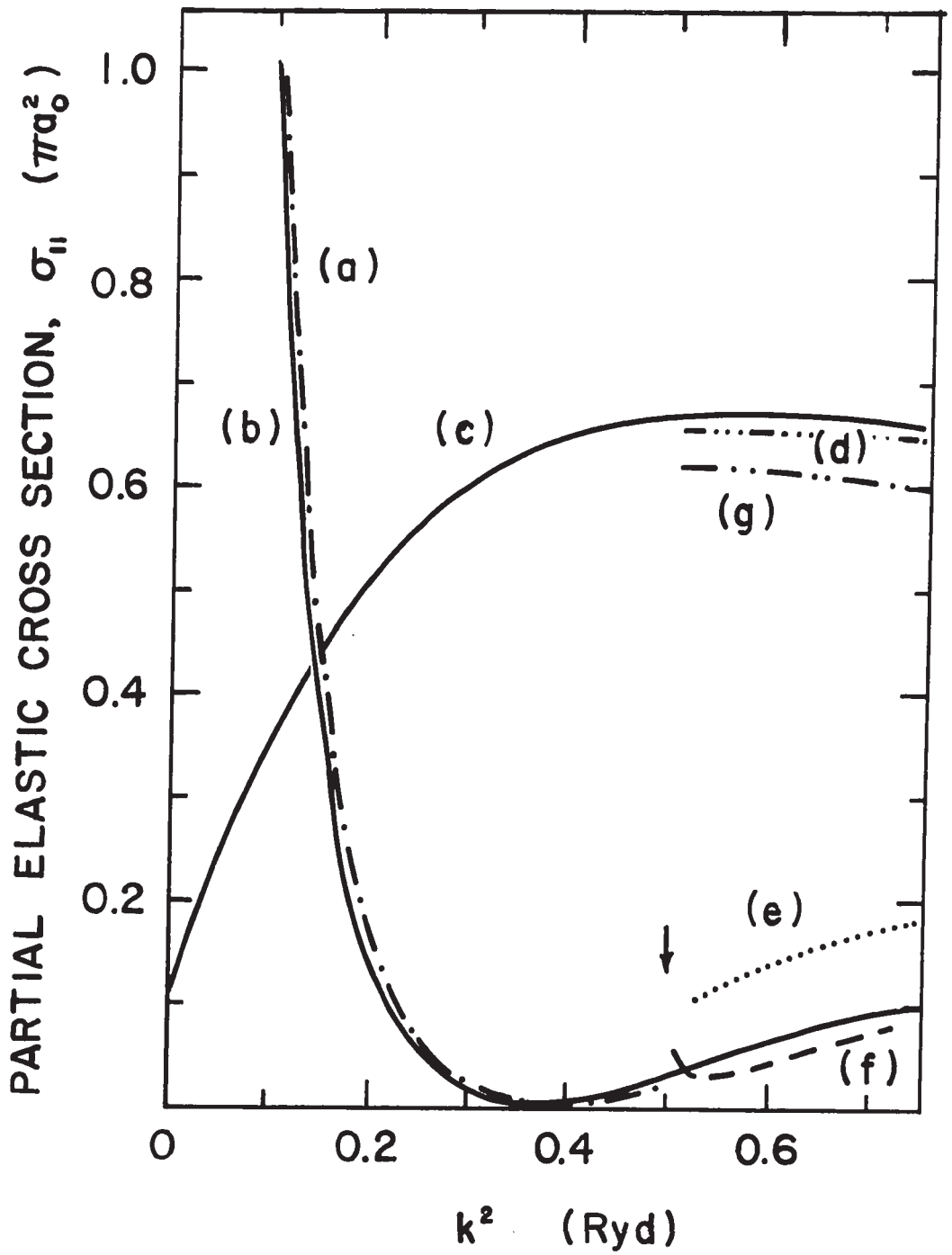

Fig.II S-Wave Partial Elastic Cross Sections. (a), Bhatia et al[1]; (b), present calculation; (c), coupled static; (d), Wakid and LaBahn[32], (their approx.(e)); (e), Dirks and Hahn[41]; (f), Bransden and Jundi[36], (their approx. B(1)); (g), Fels and Mittleman[38], (their model V). The arrow indicates formation threshold.

Positronium formation cross sections σ_{12} from this work and other calculations are plotted in Fig.III. Here, one is amazed by the diversity of the results from different calculations. Cross sections of the present result, curve (a), are more than twice as big as those (curve (d)) of Fels and Mittleman[38] (their model (V)); Dirks and Hahn[41] give cross sections (curve (d)) considerably lower, they also possess a hump at $k^2 = 0.7$. Cross sections from Bransden and Jundi (their approx. B(1)), shown in curve (f) are two orders of magnitudes higher and show a pronounced peak just above threshold. The pseudo-state expansion results of Wakid and LaBahn (their approx. (e)) are shown in curve (e). They show considerable variation in this energy region, and are much higher than the present calculation.

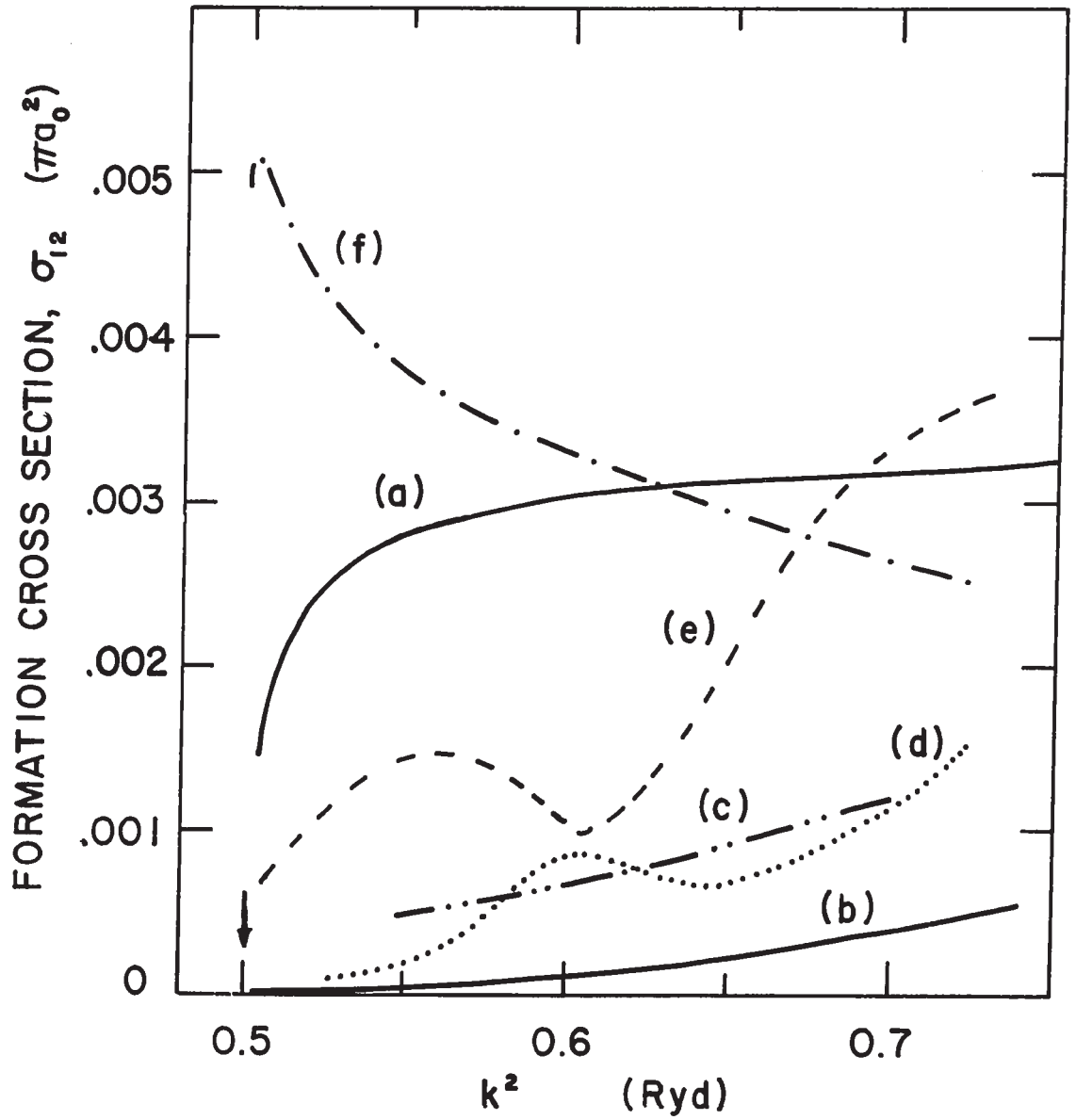

Fig.III S-Wave Partial Positronium Formation Cross Sections. (a),present calculation; (b),couple static; (c),Fels and Mittleman[38],their model V; (d),Dirks and Hahn[41] x 10; (e),Wakid and LaBahn[32], their approx.(e) x 10^{-1}; (f), Bransden and Jundi[36], their approx. B(1) x 10^{-2}. The arrow indicates threshold.

Z_{eff}

Once the functions f and g and the coefficients c_i are solved, the annihilation rate parameter Z_{eff} is calculated from (3.10) for each energy. Its values are presented in Table VI below. In the other works on this problems mentioned earlier, no calculation of this parameter has been reported. It may be due to the fact that no experimental work has been done or would be carried out in the very near future for this theorectically-simple-to attack system. Humberston and Wallace[66], in their recent detailed investigation on this problem at zero and positive energies have obtained at zero energy a $Z_{eff} = 8.9$ from their trial wave function. The present calculation gives a value of 7.65 at the same energy. Fig. IV shows a plot of Z_{eff} against k^2 showing our results and those of Ref.(66).

TABLE VI

Z_{eff} at Various Energies

k^2	0	.01	.04	.16	.25	.36	.49
Z_{eff}	7.65	6.64	5.09	3.10	2.54	2.14	1.85

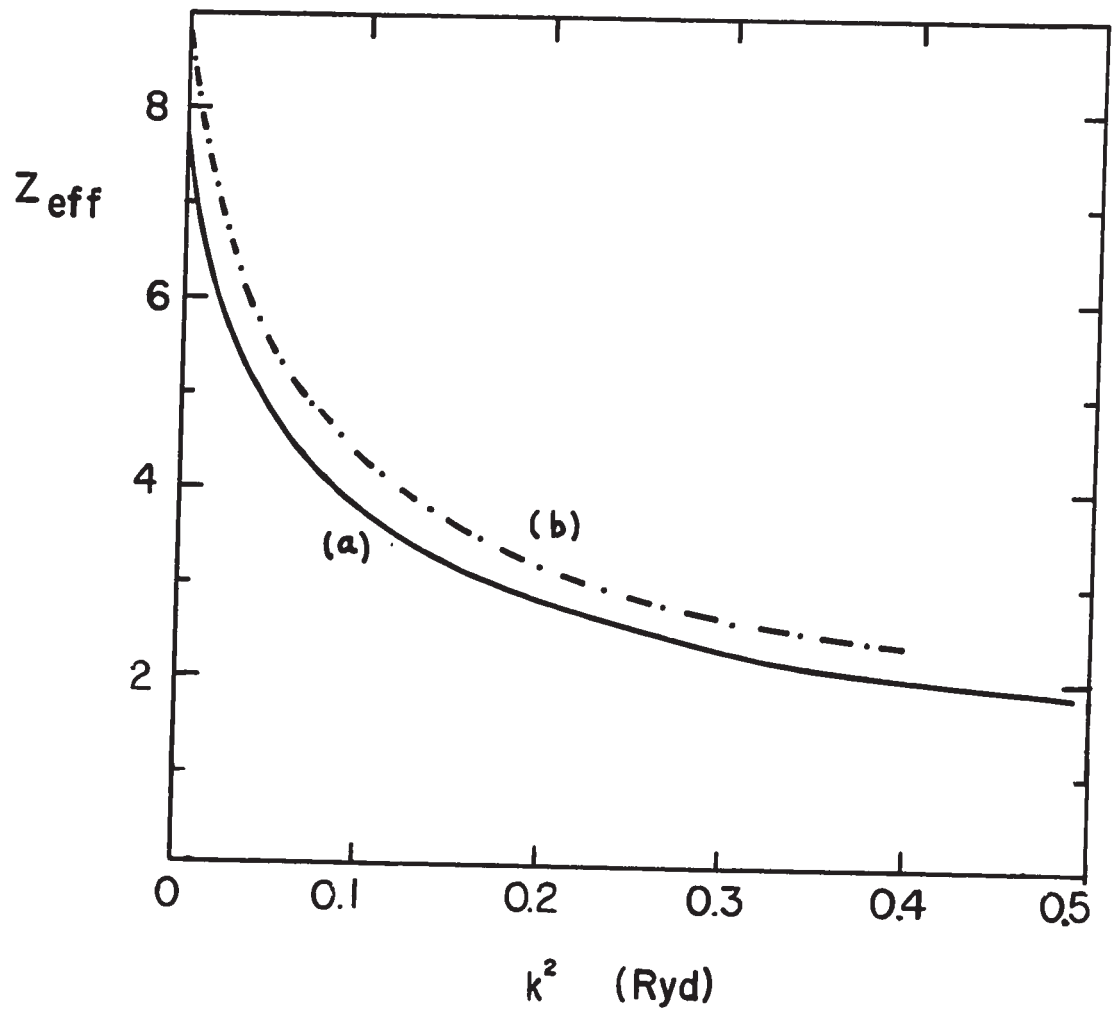

Fig.IV S-Wave Contribution to Z_{eff}.
(a),present calculation; (b),Humberston and Wallace[66].

Check on Accuracy

A check on the solution of the eigenvalue equation (2.22) is made by substituting back the eigen vector $\bar{a}^{\lambda}$ and the eigenvalue ε^{λ}into the equation $\tilde{H}\bar{a}^{\lambda} = \varepsilon^{\lambda}\tilde{N}\bar{a}^{\lambda}$. The difference between the left and right hand side for each element is always less than 10^{-6} of its absolute value. Similarly, a back substitution check on the solution of the system of linear equations gives residues less than 10^{-10}.

Table VI shows some R-matrix elements to reveal the degree of symmetry. Shown in (b), the off-diagonal elements R_{12}^{cs} and R_{21}^{cs} of the coupled static approximation are equal to within 0.2%. This remarkable agreement reflects the accuracy in numerical work involved in the two integrals of the two Green's functions with the kernel $\mathcal{K}_{12}^{cs}$, and the accuracy of the solution of the system of linear equations. However, when the correlation terms are added, (a) in Table VI, the agreement is not as good. They are within 2% of each other. The increase in discrepency may stem on the fact that some of the $\mathcal{V}_i(r_p)$ are rather long ranged, and the integration formula used does not cover the range adequately.

The other check on the numerical work using the identity (4.27) is also satisfactory. In Table VI, row (c) gives the change in $R_{\nu\nu'}$ (scattering length, or tan η_0) when 26 correlation terms are added to the coupled static approximation. Row (d) presents the right side of (4.27). One can see that the agreement is again good.

TABLE VI

R-Matrix Elements to Reveal the Accuracy of Numerical Work

k		R_{11}	R_{12}	R_{21}	R_{22}
0	(a)	-1.6975			
	(b)	.1718			
	(c)	-1.8693			
	(d)	-1.8694			
.2	(a)	.18418			
	(b)	-.04726			
	(c)	.23144			
	(d)	.23141			
.6	(a)	-.00467			
	(b)	-.24633			
	(c)	.24166			
	(d)	.24165			
.71	(a)	-.06515	-.01363	-.01365	-.07923
	(b)	-.3035	-.000513	-.000512	-.2678
	(c)	.2384	-.01312	-.01314	.1886
	(d)	.2383	-.01302	-.01296	.1876
.75	(a)	-.08621	-.02516	-.02470	-.7227
	(b)	-.3231	-.00518	-.00518	-1.4858
	(c)	.2369	-.01998	-.01952	.7631
	(d)	.2368	-.01969	-.01891	.7579
.85	(a)	-.1366	-.1324	-.1315	-5.3538
	(b)	-.3674	.1035	.1035	10.196
	(c)	.2308	-.2359	-.2350	-15.550
	(d)	.2308	-.2352	-.2393	-15.562

(a), coupled static + 26 corr. terms; (b), coupled static; (c) = (a)-(b); (d), right hand side of Eqn.(4.27). Values at k=0 are scattering lengths and at k=.2,.6 are tan η_0 .

Search for Resonances

Guided by the existence of the closed channel or Feshbach resonances in the electron-hydrogen scattering just below the excitation threshold, one wonders whether there would be also such resonances for the positron-hydrogen problem. Mittleman[2] has pointed out that the very long range potential coupling the degenerate 2s and 2p states of hydrogen and responsible for the observed resonances in the electron case is still present at large distances for the positron problem as well. He has predicted the existence of such resonances in the positron problem. Using three hydrogen states in the algebraic close coupling calculation, Seiler et al[43] have recently reported three of such resonances in the S-wave scattering of positron by hydrogen.

As the energy passes through a resonance position, one of the eigen phases increases rapidly by π and thus each element of the R-matrix will go through a violent change. A detailed search for resonances using the present trial wave function has been made. No violent behaviour of the R-matrix has been observed from the calculations with $k = 0.820$ to 0.866 in steps of 0.001. This corresponds to the search range from energy $k^2 = 0.6889$ right up to threshold in intervals of less than 0.002. Apart from this, a very thorough search with even smaller interval in k (0.00001 at times), centering at the lowest resonance reported by Ref.(43), has been performed. It still gives a negative result.

Failing to get a resonance despite the hunting, one would like to ask if the set of short range terms so chosen could possibly produce a resonant state at all. To answer this question, the same trial wave function (2.13) without the positronium term is used to solve the electron-hydrogen scattering problem with no exchange. Gailitis[26] has used a similar trial wave function symmetrized appropriately to obtain accurate singlet and triplet phase shift and resonances for the electron-hydrogen problem. A resonance is obtained in a position just below that reported by Burke and Schey[33] (Fig.V); but in addition, at lower energies, the calculation also produces some sharp increases in phase shifts (Fig.VI). To see further if the structures are real, a calculation using a close coupling code is done. Using three states, 1s-2s-2p, at k^2 = 0.04, 0.5 and 0.7, the phase shifts from the code are in agreement with those reported in Ref.(5). For the latter two points, an addition of π is necessary to make the phase shift change smoothly from lower energies. A five state (1s-2s-2p-3s-3p) calculation at fairly close energy intervals also shows similar structure at the low energy region (see Fig.VI). This unexpected result perhaps calls for a further thorough study of the electron-hydrogen system at low energies, especially when symmetrization of the wave function is put in.

The correlation functions so chosen in the trial wave function (2.13) have been demonstrated to be capable of producing a resonant state. The negative result of the

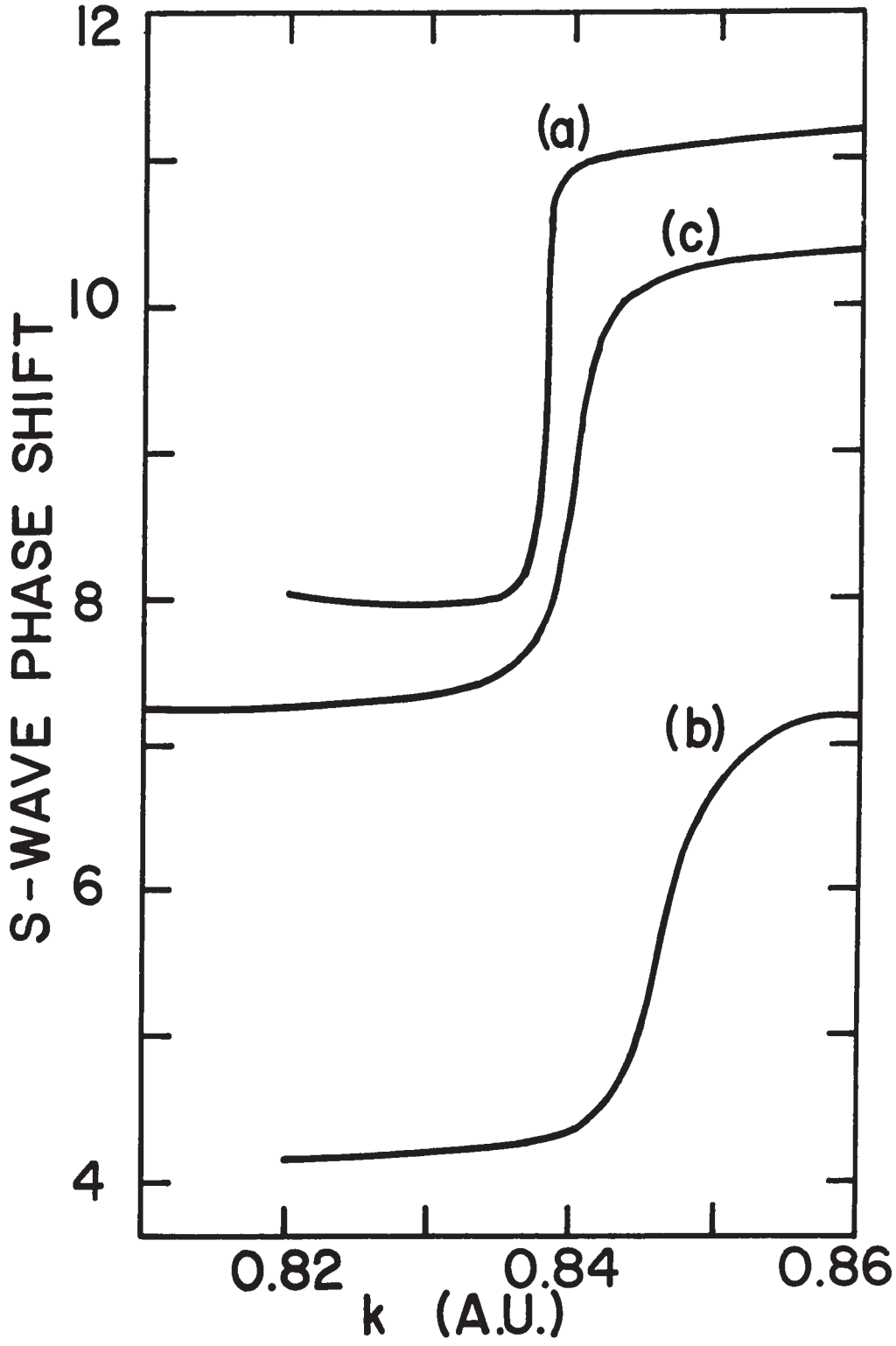

Fig.V No Exchange e^--H S-Wave Phase Shifts (A). (a), 1s + 26 corr. terms; (b), 1s-2s-2p close coupling; (c), 1s-2s-2p-3s-3p close coupling.

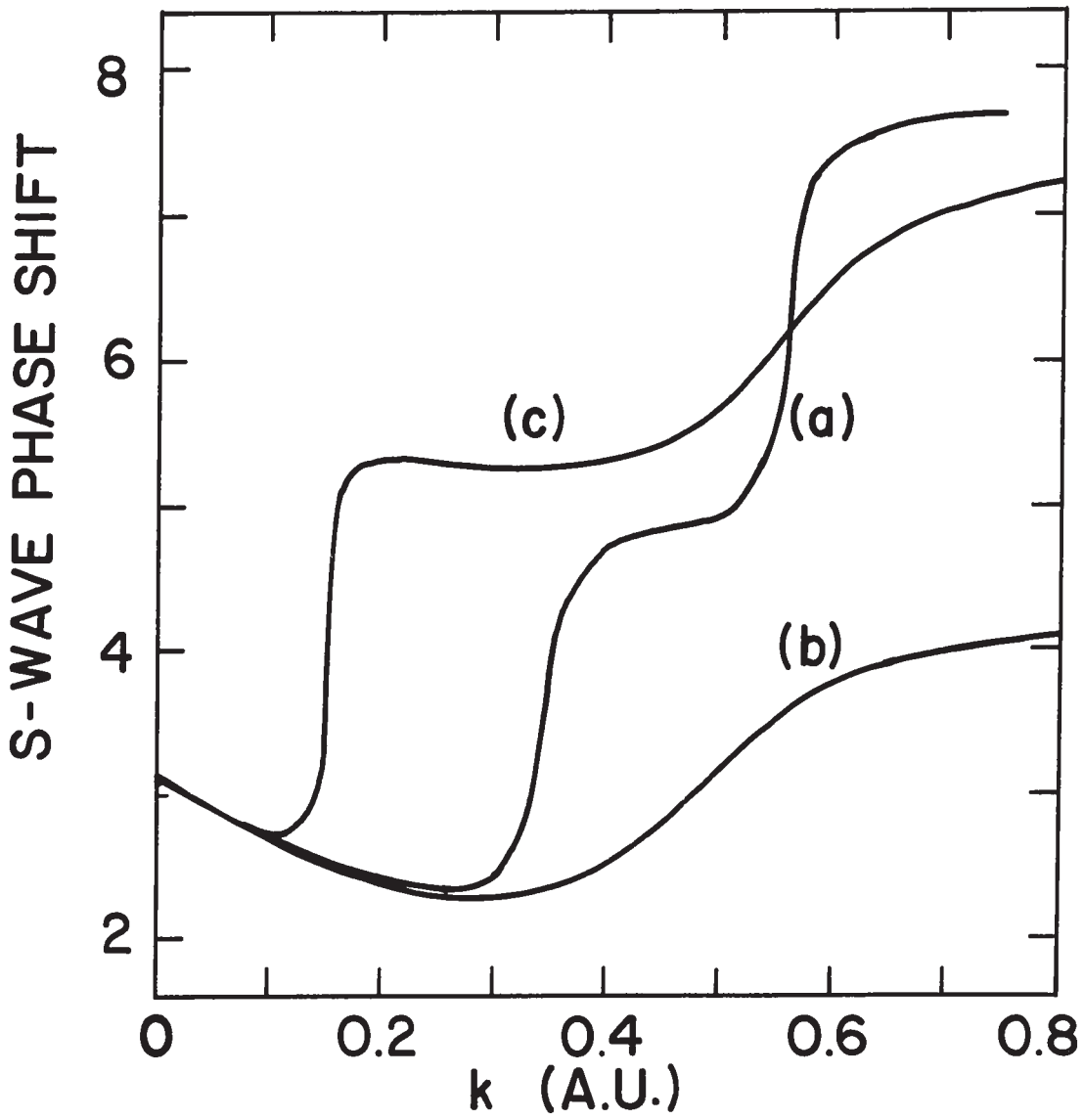

Fig.VI No Exchange e^--H S-Wave Phase Shifts (B). (a), 1s + 26 corr. terms; (b), 1s-2s-2p close coupling; (c), 1s-2s-2p-3s-3p close coupling.

resonance searching in the positron-hydrogen problem indicates that either the resonances are so narrow that they are completely missed during the search, or that there are no such resonances in the energy region under consideration.

On a closer look into the comparison of the electron- and positron-hydrogen scattering problem, one of course finds that in this energy region there is one more channel open for the latter case. Inclusion of the positronium channel in a scattering calculation may shift the observed resonances of Ref.(42) out of this energy region. Perhaps a more direct way of locating closed channel resonances is to follow the Q-operator formalism of Feshbach[39] to find the eigenvalues of the 'projected Hamiltonian' QHQ as O'Malley and Geltman[44], Temkin and Walker[67] and Bhatia et al[68] have done in calculating the autoionization states of the H^- system. The eigenvalues of QHQ below the excitation threshold are closely related to the resonances encountered in a scattering calculation.

A QHQ-calculation[69] on the positron-hydrogen problem with Q projecting out only the ground state of hydrogen has produced eigenvalues very close to the resonances reported by Seiler et al[43]. Yet, considering the positronium formation channel being open, an "increase" in the P-space will increase the eigenvalues of QHQ.

A more affirmative statement about the existence of resonances in this energy region could be made after an accurate calculation of the spectrum of QHQ, using the Q proposed by Hahn for this problem.

CHAPTER VI

CONCLUSION

This thesis represents what is believed to be the most reliable calculation to date on the inelastic S-wave scattering of positrons by hydrogen atoms. The formulation is better than many of the other reported works in that it satisfies a bound principle, and that improvement can be made systematically by increasing the number of correlation terms. One can also make the trial wave function more flexible by including a factor $\exp(-\nu\rho)$ in the correlation terms and optimize the non-linear parameters for each energy as it is done in Ref.(1).

From the work of Hahn and Spruch[22] and Bhatia et al[1] in the elastic positron-hydrogen scattering and Burke and Taylor[42] and Gailitis[26] in the electron-hydrogen system, the use of short range correlation terms to describe the closed channel wave function has been demonstrated to be very efficient. Here it has again shown its effectiveness in the positron-hydrogen system in the inelastic region.

The present calculation gives good phase shifts in the elastic region, comparable to the accurate values of Bhatia et al[1]. Further, in the elastic region, the present Z_{eff} compares well with that of Humberston and Wallace[66]. In the inelastic region, our T_{11} matrix element compares favourably with the results of Doolen et al[65]. Our diagonal

elements of the R-matrix are higher than those obtained by another lower bound calculation of Dirks and Hahn[41]. All these support the reliability of the present inelastic results.

In the absence of any experimental work and any other existing accurate theoretical calculation, as is the case here, it is very important to have a formulation that satisfies a bound principle. The algebraic close coupling method has the advantage of cutting the computation time but suffers from its lack-of-boundedness (in that the radial scattering functions are approximated by linear combination of prescribed functions). Its usefulness is also controlled by the effectiveness of the close coupling approximation. The inclusion of the polarization effects as done in Ref.(36-38) can be unsatisfactory, because it does not satisfy a bound principle, and the results depends considerably on the polarization potential chosen. There is always a danger of over-emphasizing the effect by a poor choice of potential. In the present approach, guided by the bound theorem, there is no danger of overdoing things. No matter how poorly the correlation function are chosen, the resulting diagonal R-matrix elements are always lower than the exact ones. However, some effort is of course required in finding a set of correlation functions that will give reliable results.

The difficulty to find a simple P-operator for the

positron-hydrogen problem because of the non-orthogonality of the two target wave functions in the open channels has been removed by Hahn's method of writing Schrodinger's equation in matrix form. This procedure enables us to establish the bound theorem in the way Gailitis[20] has done. The important observation of Burke and Taylor[42] in that the short range correlation terms need not be orthogonal to the open channel target wave functions saves a lot of work. One does not have to pre-orthogonalize the set of correlation terms. The work of these authors has paved the road for the present calculation.

Two methods of solutions to a system of coupled integro-differential equations have been discussed. The iterative method is simple to apply, but fails at times to converge. The latter method of converting the coupled equations to a system of algebraic equations is always applicable to solve the coupled integro-differential equations often encountered in low energy atomic collision work. The use of Gaussian quadrature in the numerical integration proves to be more efficient and time-saving than the often-used Simpson's rule. Here all the potentials and kernels vanish exponentially at large distances, and the Gauss-Laguerre formula can be used. It has helped to reduce the size of the system of linear equations to 75x75.

A detailed search for resonances using trial wave function (2.13) between $k^2 = 0.6724$ and threshold in small intervals of 0.002 has been performed and came up with a

negative result. The capability of the trial wave function to produce a resonant state has been demonstrated by applying the same 26 correlation terms to the electron-hydrogen system with no exchange. The resonances could be very narrow and may have been completely missed by our search. Alternatively, there may not be any resonances at all in the energy region we are considering. The resonances reported by Seiler et al[43] may be shifted or may disappear completely when the positronium formation channel is added to the formulation, as should strictly be done at these energies.

The question of whether or not there are closed channel resonances in the energy below the excitation threshold still has to be answered. Perhaps a direct answer is to find the lowest eigenvalue of QHQ with Q given by (2.40). It is intended that this be one of the immediate tasks to follow this thesis. It is also planned to extend the present calculation to higher partial waves.

APPENDIX A

Reduction of the Kernels K_{12}^{cs} and K_{21}^{cs} .

K_{12}^{cs} and K_{21}^{cs} are given by (2.21a) and (2.21b) as

$$K_{12}^{cs}(\bar{r}_p,\bar{\sigma}) = 8\left(-\tfrac{1}{2}\nabla_\sigma^2 - \frac{2}{|2\bar{\sigma}-\bar{r}_p|} + \frac{2}{r_p} + \frac{1}{2} - k^2\right)\psi(|2\bar{\sigma}-\bar{r}_p|)\phi(|2\bar{\sigma}-2\bar{r}_p|)$$

and

$$K_{21}^{cs}(\bar{r}_p,\bar{\sigma}) = 8\left(-\nabla_p^2 + \frac{2}{r_p} - \frac{2}{|2\bar{\sigma}-2\bar{r}_p|} - k^2\right)\psi(|2\bar{\sigma}-\bar{r}_p|)\phi(|2\bar{\sigma}-2\bar{r}_p|).$$

After performing the partial differentiations, they are both reduced to the same expression

$$K_{12}^{cs} = K_{21}^{cs}$$

$$= 8\left[\frac{2}{|2\bar{\sigma}-\bar{r}_p|} + \frac{2}{|2\bar{\sigma}-2\bar{r}_p|} + \frac{2}{r_p} - \frac{2(2\bar{\sigma}-\bar{r}_p).(2\bar{\sigma}-2\bar{r}_p)}{|2\bar{\sigma}-\bar{r}_p|\,|2\bar{\sigma}-2\bar{r}_p|}\right.$$

$$\left. - 2 - k^2\right]\psi(|2\bar{\sigma}-\bar{r}_p|)\phi(|2\bar{\sigma}-2\bar{r}_p|) \quad . \qquad (A.1)$$

In the derivation of the equation (2.27) for the functions $f(r_p)$ and $g(\sigma)$, we have to work out

$$\mathcal{K}_{12}^{cs}(r_p,\sigma) = \frac{r_p\sigma}{4\pi}\int d\hat{r}_p d\hat{\sigma}\; K_{12}^{cs}(\bar{r}_p,\bar{\sigma})$$

$$= 32\pi \frac{r_p\sigma}{2}\int_{-1}^{1} d\eta\ \psi(|2\bar{\sigma}-\bar{r}_p|)\phi(|2\bar{\sigma}-2\bar{r}_p|)\left[\frac{2}{r_p} - 2 - k^2 + \frac{1}{|\bar{\sigma}-\bar{r}_p|} + \frac{2}{|2\bar{\sigma}-\bar{r}_p|} - \frac{2(2\sigma^2 + r_p^2)}{|2\bar{\sigma}-\bar{r}_p||\bar{\sigma}-\bar{r}_p|} + \frac{6\sigma r_p \eta}{|2\bar{\sigma}-\bar{r}_p||\bar{\sigma}-\bar{r}_p|}\right]$$

$$= 8\sqrt{2}\left[\left(\frac{2}{r_p} - 2 - k^2\right)\mathcal{G}_0 + \mathcal{H}_0 + 2\mathcal{J}_0 - 2(2\sigma^2 + r_p^2)\mathcal{K}_0 + 6\sigma r_p \mathcal{K}_1\right] \qquad (A.2)$$

where $\eta = \dfrac{\bar{r}_p \cdot \bar{\sigma}}{r_p\,\sigma}$ and the functions $\mathcal{G}_\ell$, $\mathcal{H}_\ell$, $\mathcal{J}_\ell$ and $\mathcal{K}_\ell$ have been defined by Fraser[70] as

$$\mathcal{G}_\ell = \frac{r_p\sigma}{2}\int_{-1}^{1} d\eta\ P_\ell(\eta)\exp(-|2\bar{\sigma}-\bar{r}_p|)\exp(-|\bar{\sigma}-\bar{r}_p|) \qquad (A.3a)$$

$$\mathcal{H}_\ell = \frac{r_p\sigma}{2}\int_{-1}^{1} d\eta\ P_\ell(\eta)\exp(-|2\bar{\sigma}-\bar{r}_p|)\frac{\exp(-|\bar{\sigma}-\bar{r}_p|)}{|\bar{\sigma}-\bar{r}_p|} \qquad (A.3b)$$

$$\mathcal{J}_\ell = \frac{r_p\sigma}{2}\int_{-1}^{1} d\eta\ P_\ell(\eta)\frac{\exp(-|2\bar{\sigma}-\bar{r}_p|)}{|2\bar{\sigma}-\bar{r}_p|}\exp(-|\bar{\sigma}-\bar{r}_p|) \qquad (A.3c)$$

$$\mathcal{K}_\ell = \frac{r_p\sigma}{2}\int_{-1}^{1} d\eta\ P_\ell(\eta)\frac{\exp(-|2\bar{\sigma}-\bar{r}_p|)}{|2\bar{\sigma}-\bar{r}_p|}\ \frac{\exp(-|\bar{\sigma}-\bar{r}_p|)}{|\bar{\sigma}-\bar{r}_p|}\ . \qquad (A.3d)$$

The radicals in the denominators of some of the integrals in (A.3) may lead to difficulty in carrying out the numerical integration in the form they stand. This difficulty can be removed by a suitable change of variable. The following scheme is used.

We define

$$p \equiv r_p/\sigma \quad , \quad q \equiv 2\sigma/r_p \, , \quad -1 \leq \xi \leq 1 \quad .$$

For

$$0 < p \leq 1 \; : \; \eta = \frac{1}{2} p - \xi - \frac{1}{2} p\xi^2$$

$$1 \leq p < \sqrt{2} \; : \; \eta = \frac{1}{2p} - \xi - \frac{1}{2p} \xi^2$$

$$0 < q \leq 1 \; : \; \eta = \frac{1}{2} q - \xi - \frac{1}{2} q\xi^2$$

$$1 \leq q < \sqrt{2} \; : \; \eta = \frac{1}{2q} - \xi - \frac{1}{2q} \xi^2 \quad .$$

As an illustrative example, the $\mathcal{H}_o(r_p,\sigma)$ integral becomes

$$0<p\leq 1: \; \mathcal{H}_o = \frac{r_p}{2}\int_{-1}^{1} d\xi \exp[-\sigma\{1+p\xi+(2(1+p\xi)^2+2-p^2)^{\frac{1}{2}}\}]$$

$$1\leq p<\sqrt{2}: \; \mathcal{H}_o = \frac{\sigma}{2}\int_{-1}^{1} d\xi \exp[-\sigma\{p+\xi+(2(p+\xi)^2+2-p^2)^{\frac{1}{2}}\}]$$

$$0<q\leq 1: \; \mathcal{H}_o = \sigma\int_{-1}^{1} d\xi (1+q\xi) \frac{\exp[-r_p\{1+q\xi+\frac{1}{2}(2(1+q\xi)^2+2-p^2)^{\frac{1}{2}}\}]}{(2(1+q\xi)^2+2-q^2)^{\frac{1}{2}}}$$

$$1\leq q\leq\sqrt{2}: \; \mathcal{H}_o = \frac{r_p}{2}\int_{-1}^{1} d\xi (q+\xi) \frac{\exp[-r_p\{q+\xi+\frac{1}{2}(2(q+\xi)+2-q^2)^{\frac{1}{2}}\}]}{(2(q+\xi)^2+2-q^2)^{\frac{1}{2}}} \quad .$$

A 10-point Gauss-Legendre integration formula is used to evaluate these integrals.

APPENDIX B

Proof of $M^{-1} - A(AMA)^{-1}A = M^{-1}B(BM^{-1}B)^{-1}BM^{-1}$

From the definition of B = 1-A, we note

$$BA = 0$$

Let $$\alpha = M^{-1} - A(AMA)^{-1}A$$

$$B\alpha = BM^{-1} \tag{B.1}$$

$$\begin{aligned} M\alpha &= 1 - MA(AMA)^{-1}A \\ &= A + B - (AMA)(AMA)^{-1}A - BMA(AMA)^{-1}A \\ &= B(1 - MA(AMA)^{-1}A) \end{aligned}$$

$$M\alpha = BM\alpha \tag{B.2}$$

$$\alpha = M^{-1}BM\alpha$$

$$B\alpha = BM^{-1}BM\alpha = BM^{-1} \text{ , from (B.1)}$$

$$\begin{aligned} M\alpha &= (BM^{-1}B)^{-1}BM^{-1} \\ &= B(BM^{-1}B)^{-1}BM^{-1} \text{ , from (B.2)} \end{aligned}$$

therefore,

$$\alpha = M^{-1}B(BM^{-1}B)^{-1}BM^{-1}$$

APPENDIX C

To Show (2.47) and (2.19) Give the Same Equations.

To illustrate the basic arguments, let us just consider the set $\{\theta_i\}$ of two members, θ_1 and θ_2. We define

$$\Lambda^{(1)} = Q_1\theta_1 = (1 - P_1)\theta_1 = \theta_1 - \psi f_1$$
$$\Lambda(2) = Q_2\theta_2 = (1 - P_2)\theta_2 = \theta_2 - \phi g_2 \ . \qquad (C.1)$$

Because θ_i goes to zero asymptotically, we have

$$f_1 \underset{r_p \to \infty}{\sim} 0 \qquad \text{and} \qquad g_2 \underset{\sigma \to \infty}{\sim} 0 \ .$$

Our $\tilde{A}$ introduced in (2.45) now takes explicitly the form

$$\tilde{A} = \begin{pmatrix} |\psi><\psi| + |\Lambda^{(1)}><\Lambda^{(1)}| & 0 \\ 0 & |\phi><\phi| + |\Lambda^{(2)}><\Lambda^{(2)}| \end{pmatrix} .$$

Using a $$\tilde{\Psi}^t = \begin{pmatrix} \psi F + c_1\theta_1 \\ \phi G + c_2\theta_2 \end{pmatrix} \qquad (C.2)$$

equation (2.47),

i.e. $$\tilde{A}(\tilde{H}-\tilde{E})\tilde{A}\Psi^t = 0 \ ,$$

gives

$$\langle\psi|H-E|\psi F + \phi G + c_1\Lambda^{(1)} + c_2\Lambda^{(2)}\rangle = 0 \qquad \text{(C.3a)}$$

$$\langle\phi|H-E|\psi F + \phi G + c_1\Lambda^{(1)} + c_2\Lambda^{(2)}\rangle = 0 \qquad \text{(C.3b)}$$

$$\langle\Lambda^{(1)}|H-E|\psi F + \phi G + c_1\Lambda^{(1)} + c_2\Lambda^{(2)}\rangle = 0 \qquad \text{(C.3c)}$$

$$\langle\Lambda^{(2)}|H-E|\psi F + \phi G + c_1\Lambda^{(1)} + c_2\Lambda^{(2)}\rangle = 0 \; . \qquad \text{(C.3d)}$$

Using (C.1), the ket $|\psi F + \phi G + c_1\Lambda^{(1)} + c_2\Lambda^{(2)}\rangle$ can be rewritten as

$$|\psi(F-f_1) + \phi(G-g_2) + c_1\theta_1 + c_2\theta_2\rangle$$

$$= |\psi\, F' + \phi\, G' + c_1\theta_1 + c_2\theta_2\rangle$$

with $F' \equiv F - f_1 \underset{r_p \to \infty}{\sim} F$

and $G' \equiv G - g_2 \underset{\sigma \to \infty}{\sim} G$.

Equations (C.3a) and (C.3b) now become

$$\langle\psi|H-E|\psi F' + \phi G' + c_1\theta_1 + c_2\theta_2\rangle = 0 \qquad \text{(C.4a)}$$

$$\langle\phi|H-E|\psi F' + \phi G' + c_1\theta_1 + c_2\theta_2\rangle = 0 \; . \qquad \text{(C.4b)}$$

Making use of these two equations, (C.3c) and (C.3d) can be converted into

$$\langle\Lambda^{(1)}+\psi f_1|H-E|\psi F' + \phi G' + c_1\theta_1 + c_2\theta_2\rangle = 0$$

$$\langle\Lambda^{(2)}+\phi g_2|H-E|\psi F' + \phi G' + c_1\theta_1 + c_2\theta_2\rangle = 0$$

or

$$\langle\theta_1|H-E|\psi F' + \phi G' + c_1\theta_1 + c_2\theta_2\rangle = 0 \qquad \text{(C.4c)}$$

$$\langle\theta_2|H-E|\psi F' + \phi G' + c_1\theta_1 + c_2\theta_2\rangle = 0 \; . \qquad \text{(C.4d)}$$

We see that the equations (C.4) are the same as that of (2.19) by using a trial wave function

$$\Psi^t = \psi F' + \phi G' + c_1\theta_1 + c_2\theta_2$$

in Kohn's variational principle (2.16).

When $\{\theta_i\}$ has more than two members, one has to transform $\{\Lambda_\mu^{(1)}\}$ and $\{\Lambda_\nu^{(2)}\}$ into orthonormal sets. But the basic argument remains the same.

Furthermore, if we put $\theta = \theta_1 = \theta_2$ in $\tilde{\Psi}^t$ of (C.2), (C.4) will become a system of equations for F', G' and c, where $c = c_1 + c_2$. Again we have the same equation (2.19) as if we used a trial wave function $\Psi^t = \psi F' + \phi G' + c\theta$ in Kohn's variational principle (2.16). Similarly for the partitions $\{\theta_\mu^{(1)}\}$ and $\{\theta_\nu^{(2)}\}$ of $\{\theta_i\}$, the subsets can overlap. The sum of the coefficients of the overlapping members will be determined.

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